National Science Foundation

NIST National Institute of Standards and Technology • Technology Administration • U.S. Department of Commerce

INTRODUCTION

Looking for a great opportunity for your undergraduate students to get hands-on research career experience during the summer? Submit a proposal to participate in the National Institute of Standards and Technology (NIST) - National Science Foundation (NSF) Summer Undergraduate Research Fellowship (SURF) program for students majoring in science, mathematics and engineering. As of 2003 all seven of NIST's measurement and standards laboratories are participating in this exciting program: Building and Fire Research, Electronics and Electrical Engineering, Information Technology, Manufacturing and Engineering, Materials Science and Engineering, Chemical Science and Technology, and Physics.

The SURF program is designed to increase NIST's role in the training of future generations of scientists and engineers and to increase the involvement of women and minorities in science, mathematics and engineering. This program exposes students to applied research procedures in a unique environment while working one-on-one with world-class NIST scientists.

In addition to the laboratory experience, SURF seminars, extramural group activities, and an end-of-the-summer SURF Symposium enhance the students' experience. The SURF seminars feature lectures by leading industrial researchers, academic leaders, and world-class NIST scientists that expose the students to a variety of research applications. At the end of the summer, the students feel pride and a sense of accomplishment as they participate in the SURF Symposium. This symposium provides an opportunity for the students to present their summer work before their fellow SURF students and the NIST scientific community in a conference-like setting. During the following school year, students are strongly encouraged to present their research results at national meetings. This book provides you a glimpse of the 2003 SURF program at NIST from the schools and students involved, student activities, seminar speakers, and an abstract of the final student presentations. We hope that by reviewing this information you will consider joining us in this exciting program.

http://www.surf.nist.gov/surf2.htm

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The Summer Undergraduate Research (SURF) Program at NIST

The National Institute of Standards (NIST) and the National Science Foundation (NSF) are committed to the development of undergraduate students interested in exploring research careers. The Summer Undergraduate Research Fellowship (SURF) program is a NIST-NSF partnership that provides opportunities for students to actively participate in NIST research programs. The SURF program, which began in 1993 in NIST's Physics Laboratory (PL), has now expanded to include all seven of the NIST laboratories, i.e., Building and Fire Research Laboratory (BFRL), Electronics and Electrical Engineering (EEEL), Chemical Science and Technology (CSTL), Information Technology (ITL), Manufacturing Engineering (MEL), and Materials Science and Engineering. SURF is a part of the NSF Research Experiences for Undergraduates (REU) Program.

The SURF program is designed to increase NIST's role in the training of future generations of scientists and engineers and to increase the involvement of women and minorities in science, mathematics and engineering. The goal of this program is to expose students to applied research procedures in a unique environment. In addition to the laboratory experience, several additional components of the program are designed to enhance the students' experience.

Citizenship Requirements
The program is open to all United States citizens or permanent residents.

Student Eligibility
Students should be undergraduate students with a scientific major, a G.P.A. of 3.0/4.0 or better, intend to pursue a Ph.D., and must be covered by a health insurance plan (either through school or family). Students with physics, material science, chemistry, applied mathematics, computer science, or engineering majors are always encouraged to apply. However, there may be research opportunities for students with other majors.

Living Arrangements
SURF students participate in the SURF program at the headquarters site of the National Institute of Standards & Technology (NIST). NIST is located in Gaithersburg, Maryland, about 25 miles (40 kilometers) from the center of Washington, D.C. Housing arrangements have been made with two local apartment complexes for the SURF students to share fully furnished apartments. Transportation from these apartments to and from the NIST campus will be provided.

The Washington Metropolitan area is rich in cultural and recreational opportunities. The apartments are just a short commute from the nation's capital, theaters, movies, restaurants, evening entertainment, historical and cultural sites, museums, shopping, and many local universities.

Research Programs Available to Students
As of 2003, all seven of NIST's measurement and standards laboratories are participating in the SURF programs: Physics, Material Science and Engineering, Building and Fire Research, Information Technology, Electronics and Electrical Engineering, Chemical Science and Technology, and Manufacturing Engineering. Please see the application packet, the SURF website (http://www.surf.nist.gov/surf2.htm) or the general NIST website (http://www.nist.gov) for summaries of current research opportunities.

Financial Support
SURFers receive Research Fellowships funded jointly by NIST, NSF, and their school. Students receive a $4,000 stipend for the 12 weeks ($3000 for a limited number of 9-week slots), in addition to travel and housing allowances. Universities are encouraged to share in the program in such ways as providing student credits, travel or housing allowances.

This is a competitive program that ranks and reviews both the university and student portion of the application to determine the final list of SURF awardees. In the past, the NIST SURF program has been able to support approximately 100 students.

Deadline
The deadline for receipt of applications is in February.
Visit http://www.surf.nist.gov/ surf2.htm for this years' exact date.

Application
Applications must consist of two parts: the student's university must submit a grant proposal that provides details about its academic program and nominating one (or more students). The university should submit just ONE application -- no matter the number or department from which the students are applying. Students must provide a copy of their transcripts, two letters of recommendation, and a letter of intent or personal statement. The letter should contain information that helps the review committee make an informed decision about the student such as why the student wants to participate in the NIST/NSF SURF program, and what areas of NIST research interest the student.

Specific program information and contact information for the Program Directors, and applications can be obtained from the NIST SURF website (http://www.surf.nist.gov/surf2.htm). To receive an application by mail, you may also contact:

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NIST
100 Bureau Dr., Stop 8400 (Building 221, Room B160)
Gaithersburg, MD 20899-8400
Telephone: 301-975-4200 Fax: 301-975-3038
E-mail: sweigert@nist.gov

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2003 SURF Summer Seminars and Tours

May 27 First official work day and Orientation for Session I students

May 30 "How's It Going" Rap Session

This was a general session for students to discuss their expectations and those of their advisors and to air any concerns or feedback about things to date.

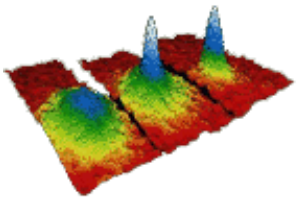
June 4 NIST Virtual Library (NVL) Demos and NIST Research Library Tour

The sessions provided an overview and tour that includes demonstrations of the Library facilities, both manual and computer-based.

June 6 Steven L. Rolston
NIST Physics Laboratory, Atomic Physics Division

Condensates, Qubits, and Quantum Mechanics

We live in a classical world, but we know that the microscopic world is described by the weird world of quantum mechanics, which allows for the possibility of an object being in two different places at the same time, for example. Some of the consequences of quantum mechanics include the existence of Bose-Einstein condensates (BECs), where many atoms coalesce into a single, identical, indistinguishable state, and the possibility of a quantum computer, a device that may out-compute any computer constructed with classical physics. Dr. Rolston discussed the work in the NIST Laser Cooling and Trapping Group to use BECs to form the building blocks of a quantum computer, confronting some of the oddities of quantum mechanics along the way.



June 10 Charles A. Wilkie
Marquette University, Department of Chemistry

Fire Performance of Clay-Polymer and Graphite-Polymer Nanocomposites

Over the past three years, our efforts have been directed in four areas: the preparation and characterization of polymer-graphite nanocomposites, on

studies that relate to mechanism of FR in nanocomposites, on the development of new thermally-stable clays and on the development of a high-throughput method to evaluate synergy with conventional FR materials. In his presentation, Prof. Wilkie addressed all of these topics.

June 11 NIST Safety Orientation for Summer Students

The session provided an overview, including how to report emergencies, use of personal protective equipment, general safety, office ergonomics, lab safety, and radiation safety.

June 12 Emil Simiu
NIST Building and Fire Research Laboratory, Materials and Construction Research Division

Chaotic Transitions in Deterministic and Stochastic Dynamical Systems: Applications of the Melnikov Method in Engineering, Physics, and Neuroscience

We describe the classical Melnikov method, a tool which provides information on the behavior of deterministic planar systems that may exhibit chaotic transitions, i.e., apparently random escapes from and captures into "safe" regions of phase space (e.g., the regions in which a boat subjected to wave excitation will not capsize). We then introduced a unified treatment of deterministic and stochastic systems that extends the applicability of the classical Melnikov method to physically realizable stochastic planar systems with additive, state-dependent, colored, or dichotomous noise. The extended method yields the novel result that motions with transitions are chaotic for either deterministic or stochastic excitation. It explains the role in the occurrence of transitions of the system and excitation characteristics, and is a powerful modeling and identification tool. We illustrate the application of the Melnikov method in mechanical engineering, naval architecture, oceanography, physics, nonlinear control, stochastic resonance, and neurophysiology.

June 13 Richard Kuhn
NIST Information Technology Laboratory, Computer Security Division

Quantum Cryptography – Today and Tomorrow OR How to Make and Break Quantum Cryptosystems (Without Being an Expert in Quantum Mechanics)

This talk provided a quick introduction to cryptography, explained why quantum cryptosystems are important, and how they work. After reviewing the basic quantum mechanisms for key generation, it was shown their use in practical cryptographic protocols, and what quantum cryptosystems exist today. Showing how to break some recently proposed quantum protocols illustrated the difficulties of doing crypto protocols right, but also provided a better understanding of their properties. The talk concluded with the discussion of possible real-world uses for quantum cryptographic products.

June 16 First official work day and Orientation for Session 2 students

June 24 Human Robot Interaction
Information Technology Laboratory

During their stay at NIST, SURFers had a chance to participate in a 45-minute experiment on human robot interaction. Each participant was asked to fill out a questionnaire and interact with a robot. The experiment was to determine what information users need to effectively and efficiently interact with robots and the design evaluation methodologies to determine if the necessary information is presented appropriately.

June 24 Evangelos Manias
Pennsylvania State University, Department of Materials Science and Engineering

Approaches for the Design and Quantitative Characterization of Challenging Polymer/Clay Nanocomposites

Melt processable polymer/clay nanocomposites have been realized for a very wide range of polymers. Two classes of polymers still provide challenges in achieving high performance hybrids composites: apolar polymers, such as polypropylene, and high-temperature polymers, such as syndiotactic-

polystyrene. The approaches we developed to address the distinctly different challenges in these two cases of polymers will be presented, including approaches involving functionalization of the polymers and ones involving non-traditional modifications for the clay fillers. Examples of materials properties and examples of TEM methodologies to quantify the dispersion of the fillers will also be presented.

June 24 Frank Gayle
NIST Materials Science and Engineering Laboratory, Metallurgy Division

Analysis of Structural Steel in the NIST World Trade Center Investigation

Last year the National Institute of Standards and Technology became the lead agency in an investigation of the World Trade Center (WTC) disaster.

The investigation addresses many aspects of the catastrophe, from occupant egress to factors affecting how long the Twin Towers stood after being hit by the airplanes, with the goal of gaining valuable information for the future. A major part of the investigation is the metallurgical analysis of structural steel from the Twin Towers. The analysis includes characterization of mechanical properties, failure modes, and temperature excursions seen by the steel. This talk on the metallurgical investigation will describe the structure of the towers, steel recovered from Ground Zero, and special issues faced in the analysis of the steel.

June 25 David Newell
NIST Electronics and Electrical Engineering Laboratory, Electricity Division

The Electronic Kilogram

In the International System of Units (SI), the kilogram is the last base unit to be defined in terms of an artifact, a century-old platinum-iridium alloy cylinder. This talk will describe one effort towards a new definition of the kilogram in terms of invariant quantities, the NIST (National Institute of Standards and Technology) Electronic Kilogram project. The project uses a watt balance which measures the ratio of mechanical to electrical work, linking the meter, the artifact kilogram, and the second to the practical realizations of the ohm and the volt derived from the quantum Hall and the Josephson effects. In 1998, the NIST watt balance set an upper limit on the drift rate of the artifact kilogram of 2×10^{-8}/yr (PRL Sept. 21, '98). By using the theoretical values for the Josephson and von

Klitzing constants, the same results yield an SI determination of Planck's constant with a combined relative uncertainty of 8.7×10^{-8}, the most accurate determination to date.

June 27 Terrell Vanderah
NIST Materials Science and Engineering Laboratory, Ceramics Division

Talking Ceramics

In the last three decades communications technologies have been completely transformed by the "wireless revolution." Devices such as cell phones are now so common that many consumers are forgoing the hard-wired versions altogether. Yet, this remarkable technological explosion could not have taken place without several key historical events, such as Marconi's first wireless transmission across the Atlantic Ocean in 1901, and the discovery of the transistor almost 50 years later. Also critical was the discovery of a small number of enigmatic ceramic materials with unique properties permitting them to be used as "dielectric resonators" and filters; i.e., "talking ceramics," which were the subject of Dr. Vanderah's talk.

June 30 NIST Safety Orientation for Summer Students – 2nd SURF Group Entrance

The session provided an overview, including how to report emergencies, use of personal protective equipment, general safety, office ergonomics, lab safety, and radiation safety.

July 2 Daniel Krieger
Goddard Space Flight Center,
Equal Opportunity Office

NASA Research Center Tour

Through a former SURF student now at NASA, 25 SURF students were able to visit the NASA Research Center and attend a talk on the NASA Mars Program. Due to the popularity of the tour, a lottery was necessary to pick the 25 "winners" who were able to attend the tour.

July 3 Ted Vorburger
NIST Manufacturing Engineering Laboratory, Precision Engineering Division

Bullet Metrology for Crime Scene Investigation

Bullets and casings, when fired or ejected from guns, pick up characteristic surface markings that are unique to the weapon. By analyzing these signatures, firearms examiners can connect a particular firearm to criminal acts. Automated optical inspection systems linked to large databases greatly aid these ballistics investigations by performing the tedious job of down-selecting the likely candidate matches for the examiners to inspect manually. We have developed standard bullets and prototype standard casings to help verify that these optical systems are operating properly. We will first describe case studies showing the successful use of the optical inspection systems to solve violent crimes in several U.S. cities and then describe the standard bullets and casings, how they are manufactured, and their intended use.

July 8 Frederick W. Mowrer
University of Maryland, Department of Fire Protection

Geometric Effects on the Fire Resistance of Structural Steel Elements

Standard methods have been developed and are used in current design practice to determine by calculation the fire resistance rating of structural steel elements protected with spray-applied fire resistive materials (SFRMs). These calculation methods are based on simplified analysis of heat transfer through the SFRM material to the steel substrate. This analysis assumes one-dimensional heat transfer in Cartesian coordinates. Based on this analysis, the ratio of the volume per unit length to the surface area per unit length, expressed in terms of the "W/D ratio," is the governing parameter for the steel element. For cylindrical elements, such as the steel rods in the floor joists of the World Trade Center twin towers, this analysis is inappropriate because of the increasing surface area of the insulated element with increasing insulation thickness. Numerical heat transfer analyses have been performed in both Cartesian and cylindrical coordinates that demonstrate the reduced fire resistance associated with a given thickness of insulation on a cylindrical rod relative to a flat element with the same W/D ratio. As the thickness of insulation is increased, the relative fire resistance rating of the cylindrical element diminishes further with respect to the planar element. The assumption and bases for these

numerical heat transfer analyses are described along with the results of these calculations, which demonstrate the importance of these geometric effects on the fire resistance of structural steel elements.

July 11 Dan Madrzykowski
Building and Fire Research Laboratory, Fire Research Division

Fight Fire with Research

Each year approximately 4,000 people die and 23,000 people are injured due to fires. In addition, on average 100 firefighters die and more than 80,000 firefighters are injured in the line of duty. The Fire Research Division at NIST is using a wide range of methods, from computational fluid dynamics to instrumenting buildings and burning them down, to develop a better understanding of fire and how to protect people from it. This presentation focused on the research being conducted to improve firefighter safety. NIST, in cooperation with the U.S. Fire Administration, is investigating new test methods for firefighter protective clothing, thermal imaging cameras and Personal Alert Safety Systems (PASS). NIST is also working with the National Institute of Occupational Safety and Health (NIOSH) to understand the fire behavior when firefighter line-of-duty deaths occur. NIST-developed computer models, FDS and Smokeview, can provide insight into "real" fires with results that can show how the fire behavior may have led to the fatalities.

July 16 Jordan Goodman and Michael Coplan
University of Maryland

University of Maryland Graduate Program

Dr. Goodman, chairman of the UMD Physics Department, and Dr. Coplan, director of the UMD Chemical Physics Program, spoke about their department/program and the research done at the University of Maryland. This was followed by a discussion of graduate school in general, and applying to graduate programs in particular.

July 18 Michael Vecchione
Smithsonian Institution, National Museum of Natural History

Weird Deep-Sea Squids and the Nature of Natural History

The recent report in the journal ***Science*** (**294**, 2505 (2001)) of unusual squids that have been encountered in very deep waters around the world has generated considerable interest by the press and the public. These sightings highlight how little is known about life in the largest ecosystem, by far, on earth. These findings provide a good example of the importance of basic observations in advancing scientific knowledge.

July 21 NASA REU Program Visit to NIST

On July 2, about 25 SURFers toured the NASA facilities and invited their counterparts at NASA to check out NIST. Thirty-five students from the NASA REU program toured the nanomagnetism, calibration support for NASA's Earth Observing System, integrating sphere-based UV chamber, and the 3D testing device labs.

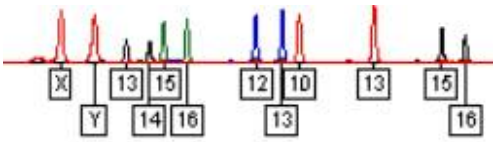
July 22 Bradley A. Williams
Naval Research Laboratory, Navy Technology Center for Safety and Survivability, Combustion Dynamics Section

In-situ Optical Diagnostics in Real-Scale Fire Tests: Capabilities and Implementation

Large scale fire tests present challenging problems of achieving measurement of a number of factors, including temperature, concentrations of fuel, oxygen, gaseous suppressants, suppression by-products (e.g., hydrogen fluoride for fluorocarbon suppressants), and number densities and sizes of particles or droplets of condensed phase suppressants. In their fire test facility in Chesapeake Beach, MD, they have tested a number of suppression concepts and configurations in enclosed chambers ranging from 1000 ft^3 to 10,500 ft^3, simulating shipboard flammable liquid storerooms. In these tests we have used three in situ diagnostic instruments, hardened to withstand the fire environment. Fourier Transform Infrared Spectroscopy is used to determine concentrations of fluorocarbon suppressant, hydrogen fluoride and carbonyl fluoride by-products, as well as carbon monoxide and dioxide, and fuel and water vapor. For determining oxygen concentrations we have developed a laser diode based sensor, able to measure an absolute O_2 concentration directly, free from corrections for water vapor or liquid

water. Finally a commercial laser-based instrument for direct imaging of particles and droplets gives critical information about condensed phase suppressants. Our approach to optical diagnostics differs from that taken by most other laboratories in that we have employed these diagnostics in-situ, rather than as part of an extractive system. Advantages and trade-offs between these two approaches will be discussed.

July 25 Peter Vallone
Chemical Science and Technology Laboratory, Biotechnology Division



Forensic DNA Typing: Application to Mass Disaster Investigations, Paternity Testing and Human Identification

Over the last 10 years DNA testing has become increasingly popular for human identification purposes. DNA typing is commonly used for paternity testing, identification of mass disaster victims and forensic human identification. The primary role of DNA typing experiments is to differentiate between individuals based on their genetic blueprint. Typically, 10 to 15 autosomal genetic markers known to exhibit variation in the human genome are probed. With current forensic testing methods the probability of a random match between two unrelated individuals is up to 1 in 3 trillion. The use of polymerase chain reaction (PCR coupled with high throughput instrumentation has enabled researchers to type sub-nanogram (a blood spot the size of a pinhead) quantities of DNA in approximately 5 hours. DNA tests are continually evolving. Currently in development are assays that exhibit greater sensitivity as well as gender and species specificity. At NIST we are providing standards for forensic laboratories, developing new DNA typing technologies, and evaluating novel genetic markers to assist the forensic community.

July 29 Marc F. Desrosiers
Physics Laboratory, Ionizing Radiation Division

Anthrax in the Mail: NIST Calibration Services to the Rescue

Scientists in the NIST ionizing radiation program played a critical role in the government's response to the past anthrax attacks. Under the direction of the Office of Science and Technology Policy, NIST led the multi-agency technical task force (U.S. Postal Service, Department of Defense, Department of Energy, Food and Drug Administration, and the U.S.

Department of Agriculture) and facilitated the adaptation of current irradiation technology to decontaminate the U.S. mail. High-energy x-ray and electron beams are proving to be effective in eradicating anthrax in contaminated mail. The talk detailed the fundamentals of this technology, as well as chronicled NIST's efforts to alleviate this problem. NIST's role in new Homeland Security projects was also presented.

July 30 David Blackburn
Electronics and Electrical Engineering Laboratory, Semiconductor Electronics Division

The Future of Semiconductor Micro/Nano Electronics

Since their invention in the middle of the 20th century, the transistor and the integrated circuit have led almost continuous revolutions in communications and computing. This has all been made possible by remarkable advancements in the science and engineering of the transistor and the IC itself. Today, there are serious concerns that fundamental physical limits and manufacturing cost will bring these advancements to a halt. The talk looked at the science and engineering of the Metal-Oxide-Semiconductor Field-Effect-Transistor (MOSFET), the heart and brain of today's ICs, and how it's continual shrinking has made the communications and computing resolutions possible. Potential roadblocks to continued shrinking were discussed, and the talk concluded with the micro/nano electronics industry's visions of the future 'transistor' and EEEL's response.

August 1 Mr. Donald Swenholt
Donald Swenholt Associates, Inc.

Giving Successful Presentations

Mr. Swenholt presented a few techniques and up-to-date procedures to assist the students in presenting their talks for the end-of-the-program SURF student symposium.

August 5 University of Maryland, College Park Tour

A number of SURFers toured the Physics, Chemistry, Electronics & Electrical Engineering, and Computer Science departments at the University to check out the possibilities.

August 6 Pentagon Tour

The SURFers had the great opportunity of touring The Pentagon. The tour route was approximately 1 1/2 miles in length and lasted for about 90 minutes. The tour covered about 20 items of interest that included the mission of the Department of Defense and each of its branches of services, and numerous displays that highlighted and depicted significant moments in military history.

August 7 Drs. Fahim Sadek and Michael A. Riley
Building and Fire Research Laboratory, Materials and Construction Research Division

Database-Assisted Design for Wind Effects on Structures

The presentation introduced the concept and applications of database-assisted design (DAD) for wind loading on low- and high-rise buildings. Historically, standard provisions for wind loads on buildings have been based on summary tables or plots suitable for slide rule calculations. The accuracy inherent in these methods is far lower than that of current methods used for stress computation. DAD allows engineers to use a database of existing wind tunnel pressure data, along with user-friendly software tools, to accurately predict the wind loads on a building. The presentation detailed the use of DAD, and demonstrated software developed at NIST for the purpose of demonstrating the capabilities of this new design approach. The results of on-going research shows that significant improvements in the main wind-load resisting system and component design can be achieved by using DAD and associated structural reliability tools, thus accounting realistically for the complexity of the wind loading as well as for the stochasticity and knowledge uncertainties affecting wind effects calculations. In the presentation DAD's capability to obtain, for the first time in a wind engineering context, realistic estimates of ultimate limit states due to local or global buckling failure were illustrated. It was shown that DAD is ideally suited for use with data likely to be obtained in the future by Computational Fluid Dynamics methods. The need for assuring quality control procedures for wind tunnel testing so that inter-laboratory comparisons of test results and wind tunnel certifications can be conducted effectively were discussed.

August 11 Final Presentations by SURF Students moderated by invited guests

August 11 Lunch with special invited guests

August 12 Final Presentations by SURF students moderated by invited guests

August 13 Final Presentations by SURF students moderated by invited guests

August 14 Final Presentations by SURF students moderated by invited guests

August 15 Last Day for SURF students

2003 SURF Summer Activities

All work and no play…not these SURFers. They work hard on their research projects all summer, but when the "whistle blows" look out for some major fun activities to balance everything out because there's always fun and adventure when you get these SURFers together.

June 25 SURF Picnic – NIST Picnic Grove

The SURF Directors provided the burgers, salads, snacks, and sodas. The SURF students were responsible for the entertainment, Frisbees, music, etc.

July 1 Camden Yards, Baltimore, MD – **GO ORIOLES!!**

Take me out to the ball game,
Take me out with the crowd.
Buy me some peanuts and Cracker Jack,
I don't care if I never get back,
Let me root, root, root for the home team,
If they don't win it's a shame….

A group of SURFers enjoyed a game of baseball between the Baltimore Orioles and the New York Yankees. The SURFers got to see the "home team" win (Baltimore 7, Yankees 3).

July 3 2003 SURF T-Shirt Design

It has become a "tradition" each year for the group to design a T-shirt during the summer. With help from Beamie Young, our resident graphics artist, this is the winning design for summer '03. There is always a huge demand for the T-shirts -- even non-SURFers want to sport them around the campus -- maybe we're talking collectors' items.

July 4

Independence Day

For 17 long, summer days in Philadelphia, a young man from Virginia worked tirelessly to draft the document that would ultimately revolutionize the world. With a quill pen and a bottle of ink, Thomas Jefferson wrote and rewrote the words that became the Declaration of Independence.

SURFers headed to the National Mall in DC to celebrate our Nation's birthday. Nowhere is there greater excitement on America's birthday than in the Nation's capital.

"Thus may the 4th of July, that glorious and ever memorable day, be celebrated through America, by the sons of freedom, from age to age till time shall be no more. Amen and Amen." Virginia Gazette on July 18th, 1777

July 12

White Water Rafting and Hiking

This year a group of 50 SURFers went white water rafting on the spectacular Shenandoah River. The group was guided through White Horse Rapids, down the famed Shenandoah Staircase, and even over Bull Falls. They floated right by historic Harpers Ferry, scene of John Brown's famous raid and many Civil War battles. As if that wasn't enough excitement several SURFers decided to hike the Maryland Heights Trail. The first part of the trail combined some steep climbs and rocky terrain but it was worth it to see the spectacular overlook of Harpers Ferry, and the Potomac and Shenandoah Rivers. The second part of the hike included much history. The trail climbed to the ridge passing remains of fortifications built by the Union forces in 1862 after their defeat at Harpers Ferry.

July 26 Old Rag Mountain Hike

Several SURFers were up for the rock scramble from one of the best hikes in Virginia. Old Rag Mountain is one of the highest peaks (3291 feet) in the Blue Ridge Mountains in northern Virginia. Old Rag's attractions include a rugged scramble over and through boulders on the Ridge Trail and a spectacular view of the Piedmont to the east and the Shenandoah Valley to the west.

July 27 Legg Mason Tennis Classic
William H. G. Fitzgerald Tennis Center, Washington, DC

The 10th Legg Mason Tennis Classic has become a 'can't-miss' event for thousands of Washingtonians. This included a group of SURFers who decided they couldn't miss the chance of possibly seeing one of their tennis favorites, such as Andre Agassi, five-time champion, or James Blake, who won his first-ever ATP title at the Classic in 2002, but alas, no Anna Kournikova!

August 9 Kings Dominion

A long-standing tradition is the end-of-the-program trip to Kings Dominion. The SURFers found the ads are true – "there really is something for everyone" from the Drop Zone to Sponge Bob Squarepants.

August 15 Last Day for SURF Students

The SURF Directors treated all 113 SURF (66 schools) students to a farewell party of pizza and soda. The party gave the students and Directors a chance to exchange plans (maybe to apply again next year), talk about their summer at NIST, and what their hopes are for their upcoming school year.

Student Abstracts from the 2003 Program at NIST

American University

Automation of Ionizing Radiation Measurements
John Patrick Casey

Current radioactivity and half-life measurements done for industry require a technician to load batches of samples and to operate the instrumentation. This is a drain on human resources for what is essentially a mundane but important task.

A computerized robotic system has been developed and built to handle 48 samples at a time, and take radioactivity measurements. The main components of the system are a Adept robotic arm, Keithley electrometer, and a PC running Labview. Samples are placed into stem holders and hung from a metal rack. Ultimately they are picked up by the robotic arm and placed into a lead chamber where a probe connected to the electrometer takes measurements. The arm is programmed separately using its own language, and then a main program written in Labview calls necessary subroutines to perform such tasks as loading and unloading samples. In the future the system is to be upgraded to handle 96 samples at a time and to operate a new chamber to handle larger samples.

Appalachian State University

An Investigation Into Current Residential Fire Codes in Regards to Safety
Matthew Cass

Today in the United States, neighborhoods are being built with houses having the minimum amount of housing separation distance between them that is allowed by current residential codes. It should be noted that the current minimum is six feet, an amount that is totally arbitrary and has no basis in scientific research. NIST was asked to investigate what the results of a fire in one of these neighborhoods would be. To do this investigation several fire-spread simulations were run using NIST's Fire Dynamics Simulator (Version 3). First, the simulator was successfully calibrated by modeling previous real life fire tests performed by the Canadians. Then the simulator was used to model different housing separation distances and see what effect, if any, these distances had on fire spread. The last simulations were of fires in a model neighborhood constructed in compliance with current national model building codes. The results of this research will be used in helping the code regulators make a decision on the safety of current residential codes.

Defining the Relationship Between Surface Composition and Protein Adsorption
Jessica Naff

The self-assembled monolayers (SAMs) of $HSCH_2CH_2CH_2O(CH_2CH_2O)_5CH_3$ were studied to further define the relationship between surface structure and protein adsorption for substrates modified with the oligo(ethylene oxide) [OEO] motif. Here we identify the boundaries between highly protein resistant surfaces (disordered = helical + nonhelical/amorphous conformations) and protein adsorbing surfaces [(a) very disordered = amorphous + exposed substrate and (b) high coverage/highly ordered 7/2 helical conformation]. To this end, the adsorption of bovine serum albumin and fibrinogen on partially and fully formed OEO-SAMs were determined. Although previous work showed that highly ordered, helical SAMs are not protein resistant, our results show that surface structure resulting in protein adsorption extends beyond this high order to include SAMs containing a moderate component of disorder, indicating that **significant** disorder is required for optimal protein resistance. Well-defined structure/function relationships on protein adsorption are key to the identification of optimal protein resistant surfaces - important to many biomedical applications such as implants, contact lenses and biosensors – as well as protein-selective surfaces. Surfaces either highly protein resistant or highly protein selective may reduce the effects of biofouling and the encapsulation process, thus increasing biocompatibility in an internal environment.

Defining the Relationship Between Surface Composition and Protein Adsorption
Erin Robertson

The self-assembled monolayers (SAMs) of $HSCH_2CH_2CH_2O(CH_2CH_2O)_5CH_3$ were studied to further define the relationship between surface structure and protein adsorption for substrates modified with the oligo(ethylene oxide) [OEO] motif. Here we identify the boundaries between highly protein resistant surfaces (disordered = helical + nonhelical/amorphous conformations) and protein adsorbing surfaces [(a) very disordered = amorphous + exposed substrate and (b) high coverage/highly ordered 7/2 helical conformation]. To this end, the adsorption of bovine serum albumin and fibrinogen on partially and fully formed OEO-SAMs were determined. Although previous work showed that highly ordered, helical SAMs are not protein resistant, our results show that surface structure resulting in protein adsorption extends beyond this high order to include SAMs containing a moderate component of disorder, indicating that significant disorder is required for optimal protein resistance. Well-defined structure/function relationships on protein adsorption are key to the identification of optimal protein resistant surfaces - important to many biomedical applications such as implants, contact lenses and biosensors – as well as protein-

selective surfaces. Surfaces either highly protein resistant or highly protein **selective** may reduce the effects of biofouling and the encapsulation process, thus increasing biocompatibility in an internal environment.

Determining Minority Carrier Diffusion Length of GaN Using Surface Photovoltage Spectroscopy

Rebecca Stamilio

Minority carrier diffusion lengths of GaN wafers and epitaxial films were measured using Surface Photovoltage Spectroscopy (SPS). While never previously employed to measure minority carrier diffusion length in nitrides, SPS is a well-established technique used with semiconductor materials such as Si and InP. Our results from GaN show reproducibility and diffusion lengths with less uncertainty than other published methods. SPS is a safe, contactless method that could save money for the semiconductor industry. Ready to process wafers utilizing GaN active regions can cost $5,000-$10,000 per wafer. If companies could characterize the quality of their materials before building semiconductor devices, they could minimize wasted time and money put into bad materials and demand higher quality from material wafers vendors.

Brown University

Analysis of Ozone-enhanced Oxidation for Device Passivation Layers

Melissa Chun

Cross-sectional analyses on semiconductor devices are important for information about electrical behavior and the fabrication process. Once a cross-section is cut, a passive layer of silicon-oxide with a thickness of 4 - 5nm is needed to preserve the fidelity of the newly exposed face. This oxide layer must be grown at a low temperature (under 300°C) in order to prevent dopant diffusion and to prevent the breakdown of the glue that is necessary to make the cross-section cut and to hold the device for measurement. Additionally, in order for an SCM (Scanning Capacitance Microscope) to get an accurate image of the cross-section, the oxide must be smooth and have good C-V characteristics.

Ozone-enhanced oxygen was used to oxidize silicon at low temperatures (250° - 400°C). The ozone-enhanced process produced a thicker oxide layer than can be obtained by thermal oxidation at the same temperature. By varying oxidation time as well as temperature, approximate growth rates were found. Surface roughness and MOS C-V (Metal-Oxide Semiconductor Capacitance-Voltage) characteristics of the oxide layers were measured to ensure that oxide layer would be suitable for use with an SCM scan.

EMC Threading
Patrick Riechl

The MEL division of NIST is involved in developing standards, such as STEP/NC, for open architecture control of machine tools and other manufacturing equipment. This is important to allow interoperability of manufacturing equipment and planning and design systems. NIST requires an open-source CNC software package to allow researchers to test the practical aspects of these new standards since. This package, called EMC (Enhanced Machine Controller), is being developed by a team of NIST scientists. In order to be able to test the real-life usage of the EMC software, NIST requires EMC-capable machines. A manual Sherline 4400 CNC-Ready miniature lathe was retrofitted with devices such as limit and home switches and a spindle encoder to better approximate a true, fully functional CNC lathe. Finally, further development of the EMC code was undertaken to allow threading functionality. Threading is accomplished by slaving z-axis travel to spindle rotation, where the amount of travel is modified by a certain scaling factor, called the pitch.

Bryn Mawr College

Evaluation of a Novel Moisture Transport Model for Epoxies and Sealant Materials
Mary Philip

Polymers are found in abundance throughout nature; from plants and animals to household appliances and paints. Particular interest is given to polymeric materials that comprise sealants, paints and coatings, as they protect surfaces from harsh climates, enhance appearances and modify surface characteristics.

The surface life of sealants and paints is a significant area of research as numerous companies aspire to create long lasting products with predictable service life. Previously, it was believed that ultraviolet radiation was the sole contributor to the destruction of coatings. Through experimentation, it has been concluded that moisture in addition to UV radiation caused the damage of substrates.

Several theoretical models have been developed to predict the moisture content and the spatial distribution of water based on various environmental parameters, such as the program MOIST. This model is quite complicated as it is based on the finite difference approach, which is computationally extensive and does not always lead to a solution. Recently, a simplification of this model was developed that did not rely on the finite difference approach; it is based on one-dimensional diffusion and uses the gradient of water-vapor pressure, a Visual Basic Program (mc_cg_1sb.xls).

This summer, diffusion coefficients were calculated using the simplified models. Using data previously collected on various substrates, the moisture content as a function of time was determined using MOIST. The plan was to compare the predictions from these two models, but the data available was insufficient. Therefore, an experimental program preparing new samples was initiated. Discussion of the advantages of these models will be presented.

Bucknell University

Characterization of Bioencapsulated Proteins

Matthew Paoletti

In recent years, the application of enzymatic proteins as industrial catalysts has become a widely studied field. In particular, researchers are exploring the range for which these proteins will remain catalytic under nonideal conditions, which is presently very limited. To this end, we have bioencapsulated alpha chymotrypsin within the pores of silica frameworks in order to investigate the extent that steric stabilization by the porous matrix expands the range of conditions in which the enzyme remains active. To further stabilize the protein, various sugars and polymers were covalently linked to the protein prior to bioencapsulation. The goal was to stabilize the protein at higher temperatures as well as in organic, nonaqueous media. The stability of the protein was explored by the relative rate of enzymatic hydrolysis of N-glutaryl-L-phenylalanine-*p*-nitroanilide (GPNA), which was measured by optical spectroscopy.

California Polytechnic State University - San Luis Obispo

Evaluation of (VUV-SE) Ellipsometer and Optical Properties of High-k Hafnium Aluminate Oxides

Kour Thay Chau

During my internship at SED, I have accomplished two research objectives: i) evaluating the reliability of a new spectroscopic ellipsometer, and ii) determining the optical properties of an important class of materials using this ellipsometer.
i) Instrument evaluation: a vacuum ultraviolet spectroscopic ellipsometer (VUV-SE) was recently purchased and installed at SED. In order to successfully utilize this system for material and thin film characterizations, its repeatability and precision must be established. A set of high quality SiO_2 films on silicon substrate was employed in this assessment. Each film was introduced to the system and ellipsometric data was repetitively collected for a period of time with the same conditions. The film thickness

was determined for each measurement and calculations of uncertainty and precision were determined. The results were recorded for future references.

ii) *Optical properties of high-k Hafnium Aluminate Oxides (HfAlO):* HfAlO films are of great interest in IC industry and academia as a potential candidate to replace the traditional SiO2 gates used in CMOS devices. VUV-SE measurements were performed on a set of HfAlO films, which were grown by a technique of atomic layer deposition with various Al quantities. The thickness and optical properties of the films need to be determined and correlated with the amount of Al in theses films. By using the dispersive optical function, generalized Tauc-Lorentz, we were able to model the measured data and obtain the film thickness as well as their dielectric functions (optical properties). The optical band gaps of these films are seen to vary with Al content. High Al content samples have larger band gaps indicating that by introducing the Al component in the films, one can manipulate the band gap values, which are important in device design and fabrication. The significance of this work is to demonstrate that VUV-SE technique is a robust and useful methodology tool that could be indispensable for high-k thin film research.

California State University – Sacramento

Locking to Absorption Lines for Laser Spectroscopy

Eliza Morris

The ultimate goal of this project is to determine the energy, isotope shift, and hyper-fine structure of the 3s state of atomic lithium. These properties can be determined by using Doppler-free non-resonant two-photon spectroscopy to measure the components of the 2s-3s transition. One can tune the laser to these components manually. However this method is intrinsically imprecise, as it is difficult to set the laser accurately by hand. In addition the internal stabilization system of the laser drifts as a function of temperature requiring one to constantly retune. Due to the symmetric nature of the two-photon resonance it is impossible to tell in which direction the drift has occurred. One must compensate for the drift by tuning back and forth over the peak to find the maximum. Alternatively, with an anti-symmetric line one can avoid these problems by setting to the zero-crossing point rather than the maximum. An anti-symmetric line profile can be obtained by dithering the frequency of the laser and processing the signal with a lock-in amplifier. The frequency dither is created by double passing the laser through an acousto-optic modulator. The anti-symmetric signal is then fed back to the laser to lock its frequency to the zero-crossing. By this method we are able to keep the frequency of the laser locked to the atomic transition. This will allow for accurate measurements of the 2s-3s transition in atomic lithium to be made with greater ease and precision.

Carnegie Mellon University

Creating a Web-based Aid to Monitor NIST and Customer Standards

Daniel Kim

Hundreds of customers depend on NIST's ability to maintain accurate electrical standards. As the amount of data increases, so does the need to store the data in a way that is easily accessible and prevents loss of any information. As part of an ongoing effort to maintain an up-to-date and organized record of electrical standards, a Common Gateway Interface (CGI) based webpage has been developed to aid in updating and retrieving data from the central database. In addition, users can upload their new and past records into the database in an accurate and time-efficient manner. A primary application of this webpage is to allow researchers to make accurate predications on their reference standards after seeing the trends and drift rates in their previous measurements.

Currently, the webpage has been constructed to be used for electrical standards (primarily standard resistors), but it is easily expandable to other areas. Many portions of the interface have been written to accept any generic input, allowing users to store a variety of information in a manner that is most convenient for them. The database can include as much original data as necessary for assuring the validity of tests, as well as date-stamped records of characteristics and predicted trends of NIST reference artifacts. The records in the database can be downloaded in a format that can then be used as input in other programs. This approach will help EEEL adhere to ISO/IEC 17025 requirements for assuring the quality of test and calibration results.

Polymorphic Phase Transitions in the SrO-Li_20-Nb_2O_5 System

Amanda Velázquez

Complex perovskites, ABO_3, with two or more cations mixed on the A- and/or B-sites are attractive candidates for wireless communication applications. The main structural phenomena that affect properties of complex perovskites include cation ordering and octahedral tilting. The present study focuses on these effects on the perovskite-like structures in the SrO-Li_20-Nb_2O_5 ternary system. Recently, a ternary compound $SrLi_{1/4}Nb_{3/4}O_3$ has been reported to crystallize with a perovskite-like structure. This compound was observed to exhibit three polymorphs (high-, medium-, and low-temperature) with distinct types of cation arrangement on the B-sites; however, none of these polymorphs could be sintered. The goal of the present study was to establish (i) fields of stability of these polymorphs in the ternary system SrO-Li_20-Nb_2O_5, (ii) reasons for the lack of sintering in $SrLi_{1/4}Nb_{3/4}O_3$, and (iii) structural details of the polymorphs. We used solid-state synthesis, series of quenching/annealing experiments, and X-ray powder diffraction to address the goals of this project. According to our results, both the high- and medium- temperature polymorphs can be stabilized at low (<1250˚C)

temperatures by adding $LiNbO_3$ to $SrLi_{1/4}Nb_{3/4}O_3$. All $LiNbO_3$-doped compositions could be readily sintered.

Case Western Reserve University

Optical Study of Shear-Induced Structure of Polymer-Dispersed Carbon Nanotubes

Ben Langhorst

Multi-Walled Carbon Nanotubes (MWCNT) exhibit exceptional electronic, mechanical and thermal properties and there in considerable interest in using them to make hybrid organic-inorganic materials by dispersing them in polymers. Because of their small size, however, little is known about their basic behavior, notably, how they disperse in a polymer and how these composite materials respond to an applied shear stress. Small-angle light scattering and flow birefringence were used to study the orientation of MWCNT in an elastic polyisobutylene (PIB) Boger fluid as a function of applied shear rate and confinement. The highly elastic Boger Fluid allows for strong orientation of MWCNT along the flow direction, which enables us to extract information about optical properties of MWCNT.

City College of New York – Hunter College

The Study of Nanofabricated Surfaces for Protein Immobilization

Randy Jackson

To further advance the development of new devices for biosensing, surface studies of prototype nanodevices are important. At the fundamental level, we can explore structure, kinetics and mechanisms of protein adsorption and antigen-antibody binding on different surfaces. The positioning of molecules on surfaces with nanometer precision allows us to ultimately test the limits of detection for biosensing. Our approach involves the designing of surfaces for selectivity in protein adsorption. Carboxyl-terminated thiols were positioned within alkanethiol matrices at the nanoscale, for immobilization of proteins via electrostatic interactions. Hydroxyl-terminated self-assembled monolayers have proven to be effective in resisting protein adsorption. Hence it will be used to construct the matrix into which the proteins will be patterned. The resulting patterns of carboxyl-terminated thiol molecules within the alkanethiol matrices were fabricated and characterized by atomic force microscopy. The atomic force microscopy AFM-based lithographic technique of nanografting was employed in the process of fabrication. Proteins, which are immobilized on a surface, are the sensing element in many micro array and biochip designs. In this investigation surfaces, which are engineered to contain different reactivities, are used to anchor proteins, as prototype surfaces for biosensing. Currently the conditions necessary for

protein immobilization at the nanoscale are being optimized using micro contact printing.

Clemson University

Studying Particle Release Induced by Air Jets: A Critical First Step in Explosive Particle Detection for Airport Security

Erin Ferguson

A current national priority for aviation security at US airports is the effective deployment and utilization of methods for screening passengers and baggage for trace explosive residues. Due to the low volatility of high explosives, vapor analysis is difficult and most screening methods rely on the collection and identification of explosive particles. Current methodology involves swiping suspected surfaces and the subsequent analysis of the residue on the collection swipe by ion mobility spectrometry. This approach is effective, but can only screen a small percentage of passengers. To increase the throughput of the screening process, ion mobility based walk-thru detection portals lined with an array of pulsed air jets are being tested by the Transportation Security Administration. The air jets are used to liberate explosive particles from a person with subsequent collection of the particles using one of two approaches: the human thermal plume method in which the natural convective heat plume rising above the body is used to transport the particles to a collector at top of the portal, and the "air shower" design that uses a downward directed airflow to entrain and transport the particles to a collector at the bottom of the portal. In order to determine optimal design parameters for each approach, we hope to identify what sizes of particles can be released from a test surface at varying air jet pressures and pulse durations. This is done by depositing monodisperse fluorescent polystyrene spheres in a series of sizes onto a filter or piece of cloth and exposing the sample to a pulsed air jet similar to those made for the portals. With the aid of fluorescence microscopy and particle recognition software, images taken before and after each airburst can be used to determine the number of particles released of each size. The number of particles released is plotted against the ratio of jet pressure to ambient air pressure (P/P_{atm}). Results have shown that the largest particles tested, 45 μm diameter spheres, are liberated very readily, where the smaller particles with diameters less than 10μm tend to adhere to the surfaces tested. The specific behavior of these particles, as well as other observations recorded, will be discussed in further detail.

Lightweight MgLi Alloys: The Future of Automotive Research

Katelyn Luedeke

The automotive industry is continuously looking for ways to improve their automobiles. The program entitled "Forming Lightweight Materials for Automotive

Applications" is looking to find strong, lightweight alloys that can reduce the weight of automobiles. Weight reduction in automotives can improve mileage, reduce power requirements, and increase the fuel economy.

Magnesium alloys are significantly lighter than the previously studied high strength steel and aluminum alloys. Body centered cubic MgLi alloys are only a little denser than water, making them one of the lightest alloys developed. This summer the MgLi alloys were grown into large single crystals using directional solidification in a high temperature vacuum furnace then carefully sliced using an acid saw. The sliced samples were then cleaned and polished. The polished samples were then deformed in uniaxial tension *in situ* in an optical microscope using Namarski interference. The resulting changes in surface morphology were used to explore the deformation mechanisms. The work done this summer is just the beginning of the research to be done on MgLi alloys.

College of William and Mary

A Starvation-Free Preference-Based Job Scheduler for The ScreenSaver Science Project

Samuel Small

The ScreenSaver Science (SSS) Project is an attempt to harness the power of unused computing cycles in quiescent machines to create a dynamic distributed system that does not interfere with normal machine operation. When a system becomes idle and its screen saver is launched, an SSS Server is also launched that grabs a task or unit or work from the network to be computed locally. Unlike similar projects such as Seti@Home, the SSS system is not task-specific. In other words, any application written using Java and its associated Jini and JavaSpaces extensions can be submitted to the SSS system for execution.

Currently, the SSS system uses a priority and preference-based scheme for task distribution. Each SSS Server can be configured to ask only for tasks that meet specific criteria, e.g. the specific owner or name of a computation. In this paradigm, some tasks could starve or wait infinitely long to run. We attack this problem by extending the scheduling capabilities of the SSS system and developing a multilevel feedback queue scheduler. Using this scheduler, we occasionally promote neglected or unpopular tasks to higher priority queues, thereby ensuring no task starves while preserving a system of preferential and priority-based computation. The scheduler is implemented as a stand-alone Jini service. SSS Servers receive tasks by passing preferences to the scheduler, which in return assign tasks given the preferences and parameters of the scheduling algorithm. This design allows for swappable scheduling policies and possibly dynamic (i.e. interactive) scheduling in the future.

Cornell University

Preparation and Characterization of Nanostructured Surfaces for Surface Enhanced Raman Spectroscopy (SERS)

Jennifer Robinson

As part of the Single Molecule Manipulation and Measurement (SM^3) project at NIST, this effort focuses on the structural analysis of biomolecules using vibrational spectroscopy. Surface Enhanced Raman Spectroscopy (SERS) increases the inelastic Raman cross-section several orders of magnitude, typically employing silver and gold nanoparticles in solution, thereby permitting single molecule sensitivity. Our goal is to generate nanostructured silver surfaces to support synthetic bilayer membranes, a useful model for studying the structure and function of cell membranes and its constituents, *in situ* for study via SERS.

The effect of surface structure on the size of the SERS enhancement is not well understood. Surfaces were studied to determine the relationship between physical characteristics and enhancement factors. Four preparation methods were used to generate surfaces, with the goal of a maximum enhancement factor of at least 10^6. The surfaces were prepared following previously published methods and characterized using UV-VIS and AFM techniques. Ideally, these surfaces should be quickly, easily, and inexpensively prepared, and reusable. Surface-to-surface variation as well as oxidation of the surface proved to be a source of variance in our results.

Raman microscope techniques were used to correlate structural detail with the enhancement factor. Alkanethiols were used in this study, as they form self-assembled monolayers (SAMs) with known packing densities and are often used as the tether in synthetic lipid bilayer membranes. Determination of enhancement factors on thiol-coated surfaces is straightforward compared to both thiols on nanospheres in solution and molecules on surfaces with unknown assemblies.

Davidson College

Comparison of Computational Methods for Electron-Impact Ionization Cross Sections

Gregory Scott

Electron-impact ionization cross sections are important quantities in certain areas of physical chemistry, namely in plasma modeling and mass spectrometric sampling. Accurate experimental measurements of these cross sections, however, are difficult to obtain, making necessary the use of a theoretical model. The binary-encounter-Bethe

(BEB) method produces relatively accurate predictions of the cross sections over a large energy range from a small number of quantities that can be easily generated through *ab initio,* quantum mechanical calculations. Two forms of the BEB theory have arisen that produce slightly different cross sections, one based on all-electron calculations and the other using pseudopotentials, which replace the chemically inactive core electrons in the calculations. A script has been written that generates cross sections for most molecules using both methods, based solely upon the user's input of a molecule specification. The results of these two approaches have been compared to experimental cross sections for molecules containing heavy elements, both of which produce results that fall within the experimental error of the measurements. Until more accurate measurements can be taken, neither method can be declared superior in accuracy, leading to the conclusion that the pseudopotential approach is more convenient due to its decreased cost, its elimination of empirical corrections for special cases, and its extension to systems containing atoms for which no good all-electron basis sets have been generated.

Drexel University

Automated Software Integration
Dmitriy Bespalov

Today, software integration is very expensive and complicated. It takes a lot of time and effort to integrate large-scale systems. In many cases, it is cheaper to write new software from scratch. As a result, automating this process is a very important task. Unfortunately, it is not clear whether automated integration of complex systems is even possible, because of the lack of testbeds, metrics and science.

Researchers at the National Institute of Standards and Technology have undertaken a project - Automated Methods for Integrating Systems (AMIS). This project is aimed to investigate the art and science of solving this problem. Throughout the summer, I worked on several projects that are aimed to make automated software integration possible in the future. In this presentation I will talk about the work that is occurring at NIST and its importance to automated software integration.

Semantic Integration Through Invariants
Joe Kopena

Software and knowledge integration presents a daunting challenge for a world increasingly driven by and reliant on information technology. A body of computer applications and code of ever-growing size and complexity makes connecting software to solve new problems progressively more complicated, resource-consuming, and error-prone even as it makes doing so more rewarding. Similarly, the extensive, diverse, and

expanding corpus of knowledge, information, and data available on the World Wide Web promises to raise automated agents and services to a new level of utility and capability if it could be rendered software accessible. However, reasonable approaches to attributing machine-interpretable semantics to Web content will necessitate integration of those representations.

One approach to resolving these issues is interoperation through an interlingua---exchange between integration targets is accomplished through translations to and from a shared language. By using a formal ontology as the interlingua, the targets can be characterized using invariants rigorously defined by properties of possible models of the interlingua. These characterizations leverage the structure of the domain as defined by the interlingua to enable such tasks as providing unambiguous definitions of target concepts, performing automated translation at a semantic level, compiling point-to-point mappings, coverage and interoperability analysis, and developing formal ontologies for informally specified legacy systems.

This talk presents work on generating these characterizations, developing retrofit ontologies, comparing and analyzing integration targets, compiling direct mappings, and translation through an interlingua framework based on these characterizations. Attention is paid throughout this work to supporting applications and information sources with and without an existing explicit formal ontology. Examples and demonstrations are drawn from the domain of business and manufacturing processes. The NIST Process Specification Language (PSL) is used as the interlinqua. Representative targets include: the process modeling component of DAML-S, a web services description language; IDEF3, a process modeling language widely used in industry and business; and ILOG, a commercial process planner and scheduler.

Duke University

Measuring the Neutron Lifetime Using Magnetically Trapped Ultracold Neutrons

Daphne Chang

Neutron beta-decay is an excellent medium for studying the weak interaction. An accurate measurement of the neutron lifetime is crucial in extracting parameters that characterize the weak force. So far, existing measurements have determined the neutron lifetime to be approximately 885±1 seconds. Researchers at NIST are now working to significantly improve the accuracy of this measurement by using magnetically trapped ultracold neutrons. With this technique, neutrons with a wavelength near 0.89 nm are scattered to near-rest and confined in a helium-filled trap with a depth of approximately 1 mK. As a neutron decays in the trap, the decay electron interacts with the surrounding helium and results in the emission of a pulse of

scintillation light. This pulse of light signals a neutron decay and the rate of pulses can be used to determine the neutron lifetime.

However, many factors affect the accuracy of the measurement attained through this technique. One such factor is background noise that arises from the surrounding environment. These background scintillation pulses appear identical to a decay-induced event when measured. Assembling a shield around the experimental apparatus minimizes this noise and thus will improve the measurement. Furthermore, developing a second detector whose count rate, when placed outside the primary experimental apparatus, corresponds to the background measurement in the primary detector, would allow the background noise to be compensated for and thus provide a more accurate measurement. This presentation will discuss the technique of measuring the neutron lifetime using magnetically trapped ultracold neutrons, as well as outline the attempt made to reduce and extract background noise in such a measurement.

Fordham University

Absolute Radiometry with Correlated Photons

Olivia Halt

Since detectors for measuring visible light are far superior to their infrared (IR) counterparts, it would be quite an advantage to detect IR light with visible detectors. Through the process of parametric down-conversion (PDC), this end can and has been attained. PDC occurs when photons pass through an appropriate non-linear crystal and decay into two correlated photon beams. Due to conservation of energy and momentum, knowledge of one output photon beam can predict the energy and momentum of the second. This is often referred to as phase matching. In addition to spontaneous down-conversion, that which is caused by the pump beam, PDC can be stimulated by an additional source beam positioned at the appropriate wavelength. Because photons in this process are stimulated in pairs, stimulating PDC with an IR beam will cause the correlated photon also to be emitted and in this case the photon is in the visible region.

It is through detection of this correlated photon beam that absolute radiometry of IR sources can be done with visible detectors. The ratio of stimulated PDC to spontaneous PDC allows one to calculate the radiance of the source beam, and this measurement is absolute because the amount of spontaneous PDC is a known absolute quantity. Measurements have been done up to values of 5 microns. Our current experiment works to push this limit up to wavelengths of 8 microns.

Gettysburg College

Fast Neutron Spectroscopy
William Anderson

The accurate measurement of the energy and fluence of fast neutrons at energies greater than 1 MeV remains an outstanding problem. Neutrons in that energy region have not been well characterized compared to lower energy thermal and epithermal neutrons. The existing detection techniques have significant shortcomings with regard to sensitivity and energy resolution. A new spectrometer using a LGdBO crystal has been developed to characterize fast neutron fields with energies greater than 1 MeV. The detector operates on the principle of measuring the energy from proton recoils and detecting a subsequent neutron capture on 6Li. This detector is being calibrated and characterized with NIST standard neutron sources in a room of well-known neutron background and scattering. The data being acquired by this detector will serve as a foundation for developing a next generation fast neutron spectrometer here at NIST. Such a detector will have applications in neutron dosimetry, underground physics, and homeland security.

Hamilton College

Transmittance of Fused Silica (SiO_0) Windows
Ben Auerbach

Beamline Four (BL-4) of the Synchrotron Ultraviolet Radiation Facility (SURF III) has been used to characterize detectors and optical materials in the wavelength range of 125 nm to 325 nm. Throughout the summer we have endeavored to measure the transmittance of fused silica (SiO_2) windows with an uncertainty of less than 0.5%. In order to achieve such accuracy and in attempt to understand the properties of absorption, and transmission of SiO_2 in both air pressure and vacuum, numerous aspects were studied in depth: such as Oxygen absorption of UV light, and an examination of pieces of BL-4 moving once air was removed.

Oxygen absorption of UV light was examined from 187 nm to 205 nm and was found to be dependent on air pressure; the results of this absorption are presented with a 10^{-1} uncertainty.

The spectral transmission curves obtained with several different fused silica samples show features that could be interpreted as both bulk absorption and surface absorption. Bulk absorption measurements depend on the thickness of the sample whereas surface absorption depends solely on the two surfaces. Bulk absorption measurements were made using 6 mm and 1.5 mm SiO_2 glass and the results are presented.

It was noticed that in a wavelength range of 200 nm to 250 nm results measured in near 740 torr pressure and near vacuum pressure, the regions did not match. The transmission for the two pressures could be off by ~ 0.5%. This talk will encompass the research that was conducted, the methods in obtaining measurements and outline future endeavors within this area of radiometry.

Harvard University

Temperature Gradient Focusing for the Separation of Proteins

Constantin (Ted) Malliaris

As the field of proteomics grows, the need for a fast, effective method of separating proteins increases. Isoelectric focusing, a widely used method, establishes a pH gradient to electrokinetically focus each protein at its isoelectric point. The major drawbacks of this technique are that, by nature, it is labor-intensive and difficult to automate. In addition, many proteins have a low solubility in water at their isoelectric points and tend to precipitate out of solution, thus interfering with the separation.

Temperature gradient focusing, a chemical separation technique being developed here at NIST as an alternative to isoelectric focusing, uses the temperature-dependent behavior of certain buffers to concentrate and separate analytes. An apparatus has been assembled that allows for the separation of proteins in a capillary. Test separations are being performed using green fluorescence protein, a protein that has 4 isoforms, which form distinct peaks and exhibits fluorescence easily recorded by a camera. To the capillary is attached the sample reservoir on one end, and a tube leading to a stage reservoir with variable height on the other. By changing the level of the stage reservoir, a pressure-driven flow can be varied so that the peaks are moved past the camera lens in succession. This presentation will describe studies that have been undertaken to examine the effect of variation of several parameters (such as electric field strength, temperature gradient slope, etc.) to determine the optimum separation conditions for proteins.

Iowa State University

Chemical Modification of TiO_2 Nanoparticles for the Improvement of Dispersion in Acrylic Urethane Polymer Matrices

Jason Holzmueller

The material properties of polymers are often enhanced by the incorporation of fillers to form a new composite material. Nanocomposites utilizing nanoscale fillers, such as nanoparticles, nanotubes, nanoclays, and nanoassemblies, are increasingly replacing

traditional composites or coatings in many commercial applications. However, due to the nature of nanostructure materials - interfacial behavior dominates due to the increased surface area to volume ratio – the system tends to form agglomerates and defects, which can affect optical properties and impact the performance and durability of the materials. In this project, TiO_2 nanoparticles were subjected to surface treatments of octyltrichlorosilane, dodecyltrichlorosilane, or methyltrichlorosilane, then dispersed in an acrylic-urethane polymer matrix. This surface treatment effectively lowered the surface energy of the Ti nanoparticles, allowing them to disperse more readily while retaining their optical properties. The effect of surfactant addition on dispersion was also monitored. The degree of dispersion was measured with confocal microscopy and light scattering. Silane bond formation was measured with IR spectroscopy. The gloss of the coatings was measured with Minolta multi-angle gloss meter. Optimum gloss and dispersion was found with a surface treatment of methyltrichlorosilane utilizing the hydrophobic surfactant Tamol 731A.

James Madison University

Synthesis of X-Ray Photoelectron Spectroscopy Lineshapes Using MATLAB

Jennifer Muth

X-ray photoelectron spectroscopy (XPS) is a common technique for chemically analyzing the surface of a material. A wealth of qualitative information can be collected in a relatively short amount of time with little data processing. However, historically it has been difficult to get useful quantitative information from surface analysis techniques due to many sources of uncertainty associated with determining the area under the peak. Such information would prove to be useful in the making of implants for the body, developing catalysts, and learning more about surface chemistry in general.

This summer, MATLAB 6.5 was used to simulate XPS spectra using a range of parameters that are patterned after those encountered in the lab. A Doniach-Sunjic lineshape was used to represent the basic photoexcitation process in the sample. Each lineshape was convolved in turn with a function representing an x-ray source. The results were then repeated convolved with the inelastic scattering cross sections for three materials. A constant background as well as Poisson noise was added to the spectra and further normalization was carried out.

The simulated spectra will be sent to a group of thirty scientists for further analysis. These scientists will then use one several available procedures to subtract the background in order to determine the peak intensities. Their results will be compared to the true peak intensities at NIST. This will allow for better assessment of the uncertainties in determination of peak areas.

Augmentation of Biopolymers for Tissue Engineering
Evan Schwartz

The recent development in the field of tissue engineering has focused attention on a class of polymers called hydrogels. These materials are now being incorporated into the human body as scaffolds to help regenerate damaged tissues, specifically cartilage, skin and bone. My project focuses on the creation of three different peptide-modified hydrogels using poly(ethylene glycol), alginate and elastin as the polymer backbone. Naturally occurring peptides were created artificially using an automated solid-phase synthesis process with the intention of coupling them to the hydrogels. Specific sequences (VTKFYF and VITFFSL) were created to modulate the cellular response of macrophages involved in the inflammatory response. Other sequences (VPGIG and LESLESK) allowed us to precisely control the structural properties of the hydrogel. RGD synthetic peptides made the gel highly compatible with cell surface receptors called integrins. All of these peptides were verified and characterized using MALDI-TOF Mass Spectrometry and Nuclear Magnetic Resonance (NMR) techniques. The relative concentrations of the peptide and polymer were altered in order to optimize the rheology and cellular response of the resulting polymers. Peptide-modified hydrogels hold much clinical promise in serving as implants to promote tissue regeneration.

Johns Hopkins University

An Investigation into the Corrosion Resistance of High Nitrogen Stainless Steel
Joe Lee

Any material designated for implantation in the human body, must be extensively tested prior to use. Researchers at NIST have developed a High Nitrogen Stainless Steel (HNSS) that may be a good candidate for biomedical applications. The results of preliminary laboratory evaluations and the existing literature both indicate HNSS has the requisite mechanical, and wear properties, and it also exhibits good corrosion resistance. However, additional evaluations must be performed to certify this material as suitable for implantation in the human body.

The goal of the present effort is to answer two fundamental questions: What is responsible for the dramatic increase in strength and corrosion resistance in HNSS as compared to a traditional austenitic stainless steel (i.e., is it the nitrogen content or the processing)? How well does HNSS resist the human body environment?

Corrosion is a great concern for any material in service and an aggressive environment, such as the human body, can have a considerable impact on the lifetime and

performance of an implant material. Our approach is to examine the corrosion behaviors of HNSS, a powder-processed 316 SS and an ingot-produced 316 SS in an environment more akin to the human body and also compare it to the behaviors in a reference acid solution. In addition, the human body may promote Stress Corrosion Cracking (SCC) that could also accelerate failure. The susceptibility of these steels to SCC will be evaluated by the Slow Strain Rate Tensile (SSRT) test.

My presentation will discuss the powder metallurgy process used to make HNSS and how this technique differs from traditional ingot methods used for most commercial steels. I will present how our approach of electrochemistry and SSRT experiments can address the above-mentioned questions and I will detail the significance of both the experimental techniques and the results. Finally I will suggest the additional work that must be performed before this material can be considered for an actual biomedical application.

Analysis of Cell Membrane Peptides Via Small Angle Neutron Scattering
Andrew Rockwell

The ability to detect minute differences in peptide chains is crucial to the analysis of several biological systems. In our study we looked at a particular peptide found in human cell membranes. The mutation of one amino acid in this peptide chain results in a genetic disease know as dwarfism, which is characterized by disproportionate skeletal growth resulting in small stature. The mutated peptide dimerizes in cell membrane significantly more then the normal peptide, which barely dimerizes at all. Two samples with lipid – peptide multilayers were created, one with the normal peptide and another with the mutant, to mimic the peptide's behavior in a cell membrane. Performing small angle neutron scattering will allow us to see the differences in structure associated with the degree of dimerization of the two peptides.

Kent State University

Computational Material Science Software Development
Kyle Stemen

While many academic and industrial scientists are continuously generating materials data, it is often in a custom or even proprietary format. This lack of uniformity inhibits collaboration and the lack of a machine-readable standard leaves a vast array of information currently untapped for the materials engineer. MatML was created as a standard language for describing such data. Being XML-based, it is machine-readable and, up to a point, human readable. This project involved developing an online editor for use by those without a computer science background. The editor was built using PHP (a scripting language) and automatic code generation off of the schema in a

nonspecific fashion, independent of MatML, allowing it to be easily adapted to other languages, so as to approach a generic XML editor. This project identified several opportunities for strengthening the MatML schema, which will be forwarded to the MatML Development Working Group for consideration.

A second project was the porting of OOF (Object Oriented Finite Element) from Unix to Windows. OOF is an engineering tool, developed in MSEL, to model materials. As most engineers work in Microsoft Windows environment, a port has the potential to dramatically increase the user base of the software. OOF is written in C++ and Python, both of which tend to port as well to Windows as they do flavors of Unix. The challenge was in the correct porting of the libraries to which OOF links. Some libraries already have ports, but different versions by different people with different quirks. To manage this maze of incompatibilities, Cygwin, a Linux-like environment, was used as an intermediate between Linux and Windows.

Lehigh University

Strength of Silicon in the Region of Small-Scale Flaws

Marina Chumakov

Silicon is one of the most technologically important surfaces today. There is no question that the electric properties of this material are well known. However much less is known about silicon's near-surface mechanical properties. Although there are many studies of nanoindentation of silicon being done, most of them relate to the phase transformations occurring during loading and unloading and the particular shape of the unloading curve. An important issue is the retention of strength of the device as small-scale flaws evolve in the structures.

This particular research, examining this issue, uses nanoindentation to introduce controlled flaws of ever-decreasing size into initially pristine silicon plates. Strength tests are then conducted by bonding the indented plate surfaces to a polycarbonate substrate, and then by applying a concentrated axial load at the top surfaces to induce fracture from the indentation sites. The measured strengths systematically increase with decreasing flaw size. Different behavior observed within the strength versus flaw size plot correlates with the damage modes induced by nanoindentation. Further exploration of these behaviors can benefit MEMS and NEMS devices, where the devices are subject to submicroscopic damage under long-term operating conditions from small-scale contacts.

Loyola College in Maryland

The Creation of a Successful Imaging System: A Step in Improving the Way We Study Plasma Arc Tubes

Stacey Watts

The annual cost for plasma light sources and incandescent light sources in the United States lies around 40 billion dollars, thus enforcing the importance of studying lighting, particularly high-intensity discharge lamps in order to create a better, brighter, energy efficient light source.

An optical imaging system was designed, built, and tested to for incorporation into a plasma diagnostic to study metal halide lamps. The design constraints were optimum spatial resolution with a minimum number of components. Two achromatic doublets were chosen to minimize the two most things important to us: spherical aberrations and chromatic aberrations. ZEMAX, a computer-based optical ray-tracing program, was used to test performance of the system for various free parameters. The performance was tested experimentally by using an optical test pattern and a CCD detector. A program was written in MATLAB to analyze data in terms of the Modulation Transfer Function versus spatial line frequency.

Marietta College

Corrosion as a Mechanism of Crack Tip Blunting in Glass

Seth Avery

Examination of arrested cracks in soda lime silicate glass by atomic force microscopy indicates that the cracks remain open after the load has been released. This permanent displacement of the fracture surfaces can have several possible causes, one of them being corrosion by the aqueous environment present at the crack tip during crack growth. In this study we measure the corrosion rate of soda lime glass in basic solutions as a function of time and temperature to determine if corrosion can occur rapidly enough to account for the crack opening displacement. Experimental methods will be described and results will be presented and compared with the crack opening displacements observed by atomic force microscopy. The possibility of corrosion as a mechanism for the residual crack opening in glass will be discussed.

Massachusetts Institute of Technology

Flow Simulation for the Development of Microfluidic Devices
Matthew Handler

Analysis of single and multi-component flow fluid was studied by means of flow simulation methods. The FlexPDE software package was used to simulate single-phase flow in various geometries. The purpose of this was to analyze the fluid dynamics of these geometries as a platform for liquid state material characterization in microfluidic devices. A number of 2-D and 3-D geometries were tried in order to delineate combinations of geometry and boundary conditions for which the flow type can be adjusted between shear and extension, while providing adequate flow strength. Prototype geometries, using these results are being developed and tested in our lab. An eventual goal is to simulate multi-phase flow using these geometries. To this end, a flow simulation for ternary blends in shear flows was also developed and some preliminary results are shown.

A Study of the Bystander Role in HRI
Iris Tang

In recent years, applications of robotics have been expanded to a variety of domains. Although these applications appear to be vastly different, there are essential similarities in how the robot must be able to comprehend and react to a human, and vice versa. A main goal of human-robot interaction (HRI) is to develop an intelligent robot while still accommodating the user's needs and desires. One area of study in HRI is to understand the human side of this interaction, focusing on how humans interact with robots.

As a continuing effort to develop an evaluation methodology, we conducted an experiment to investigate specifically the role of a bystander, who has no experience with the robot and needs to develop a model of the robot's behavior in order to co-exist in the same environment. In our experiment, we studied two factors, expectation and consistency, and how they influence the development of the bystander mental models. We hypothesized that people would expect the robot to behave like a dog due to its doglike appearance and that doglike sounds would make the unexpected behaviors more expected. We also looked at the factor of consistency in order to simulate how a robot might behave when its sensory information and world model is imperfect. The experiment was designed with different sets of behaviors and sounds and notions of consistency. The subjects were given questionnaires before and after their interaction to assess how well they were able to construct a behavioral model of the robot. The experiment was refined from last year's experiment, with improved sets of behaviors through experimentation, better scoring criteria, and logging of the interactions. Data from the study will be presented, as well as analysis that may lead to further research efforts to improve the evaluation methodology.

Miami (Ohio) University

Development of a Second Generation Domen-type Water Calorimeter as a Primary Standard for Absorbed Dose in a ^{60}Co Beam

Kathryn O'Connor

In order to provide a national primary standard for ionizing radiation, it is necessary to determine the absolute absorbed dose in a material due to incident radiation, where the quantity absorbed dose is the mean energy imparted to matter per unit mass of the material. Calibrations for radiation therapies are specified in terms of absorbed dose to water, a tissue equivalent substance. A second generation Domen-type water calorimeter, constructed at The University of Texas Southwestern Medical Center at Dallas, is used to measure the heat produced in the absorption of gamma rays from a ^{60}Co reference source. The nominal absorbed dose rate under the measurement conditions is approximately 19 mGy sec^{-1}, determined with a calibrated ionization chamber. This corresponds to a temperature rise of 0.25 mK per minute of exposure. The measurement of such a small change in water temperature is achieved through the use of a Wheatstone bridge aided by a lock-in amplifier. Various aspects of the water calorimeter, including fabrication of the thermistor probes, hydrogen purged high purity water, lock-in frequencies, duration of irradiations, and system stability, have been evaluated to facilitate the establishment of a new primary standard. Preliminary data have been used to assess its accuracy and precision under a given set of measurement conditions, with suggestions for future improvements.

Atomic Resolution Electromechanical Null Detection

Robert Seymour

The NIST Microforce Realization Project currently has a working electrostatic force balance with a resolution of 15 nN. An application of the electrostatic force balance is the calibration of an atomic force microscope traceable to SI units. A possible method of calibration is to measure the force of a covalent bond with an accuracy of one part in 10^3 nN. In order to achieve this accuracy the balance needs to have a resolution of 10 pN. The two methods to improve the resolution of a balance are to make the suspension weaker and to increase the sensitivity with which the null position is measured. Both methods have been employed to increase the resolution.

The new electrostatic force balance has a spring constant of 0.016 N/m. This dictates a null displacement resolution of less than 1 A. A photodetector with a split photodiode is investigated as a means to measure the deflection of the balance. A series of experiments are conducted to determine the maximum sensitivity and resolution that is achievable with this photodetector. The experiments employ several different lasers

and setups to make sensitivity measurements. The noise equivalent displacement at 1 Hz is also measured. The best results are achieved with a fiber-coupled IR laser yielding a resolution of 3 A.

Michigan Technological University

Ensuring the Consistency of World Model Knowledge in Autonomous Navigation
Justin Gillespie

Autonomous systems refer to embodied intelligent systems that can operate fairly independently from human supervision. Autonomous vehicles are a type of autonomous system, which guide themselves and maneuver around obstacles based upon information stored in their internal world model. The world model consists of two types of information: in situ knowledge, which is sensed data gathered in real-time by instruments like cameras, microphones, lasers, and radar; and a priori knowledge, which is data captured prior to run-time that is often saved in data structures, or databases.

When navigating on-road, route planning and vehicle movement are performed based upon the data contained in the world model, which may contain information regarding road pathways, lane markings, speed limits, travel hazards, or any other information necessary for on-road operation. The world model, however, becomes ineffective if the data within it is incorrect or inconsistent. Inappropriate, erratic, or possibly dangerous vehicle behavior is the likely effect of these data errors. One way to ensure the data in the world model is correct is by running a consistency checker over the world model database. A C++ consistency checker that uses SQL statements to query a world model database was developed in order to locate data errors and inconsistencies. As a result, errors within the world model can be found before the world model is used for vehicle maneuvering, helping to ensure safer vehicle operation.

Montgomery College

Determination of the PSD of Gypsum in Cement
Dafla Hiruy

For modeling the hydration of cement using software such as CHEMHYD, the Particle Size Distribution (PSD) and other properties of gypsum within a cement sample need to be known. The purpose of this project was to develop a method for measuring the PSD of the component of a powder such as cement, i.e. determine the PSD of gypsum while intermixed with the finely ground clinker. The method involves a PSD analysis instrument, based on the LASER light diffraction technique. The instrument processes

the refraction of light rays that passed through a sample suspended in alcohol to determine its PSD. By using different types of alcohol, and by matching their refractive indexes with the refractive index of one of the component, it is theoretically possible to measure the PSD of only that component while intermixed with the others components. This technique is simple and does not involve physically separating the components before measuring the PSD. Various clinkers, cements and gypsums were tested in different alcohols in order to validate this method. The results from these experiments look promising and will be discussed in my presentation.

Mount Saint Mary's College

The Ultraviolet Absorption Cross Sections of 1,5-Hexadiyne: Temperature Dependent Gas Phase Measurements

Megan Daschbach

In all combustion devices, the release of soot into the environment leads to a growing list of harmful environmental effects and severe health problems. Despite both the environmental and industrial ramifications, little is known about the mechanisms of soot formation. However, understanding the birth and growth process of soot particles is important to maintaining a balance between our oil-based economy and corrosion to our environment.

Amongst what is known about the soot formation process is the involvement of isomeric forms of C_6H_6, such as benzene, fulvene, and 1,5-hexadiyne. Such molecules are suspected to play critical roles in the beginning stages of soot formation. Because of its involvement, data on the absorption spectra of 1,5-hexadiyne was collected and its corresponding absorption cross sections were calculated. Such ultraviolet spectral knowledge is important to probing just how a particular species is formed. This information can then lead to the understanding of its role in combustion related reactions, and ultimately, is important to the overall comprehension of soot formation mechanisms.

Vacuum ultraviolet spectroscopy was used to collect the data on the 1,5-hexadiyne molecule. Its absorption cross sections have been measured as a function of temperature. The measurements were taken in the gas phase from 160-275 nm in a temperature range of 300 to 400 K. A broad absorption band was noted from 160 nm to 220 nm as well as a smaller band with a maximum at around 244 nm.

Degradation of PCBs in Marine Sediment by Electron-Beam Technology
Anna Kalema

The widespread release of polychlorinated biphenyls (PCBs) to the environment presents a challenging, complex issue due to the compounds' toxicity, environmental persistence, and cost associated with disposal. The toxic effects reside in the hydrophobic nature of PCBs, which causes the molecules to biocummuate in the fatty tissues of animals. Additionally, PCBs possess high thermal and chemical stability and do not extensively decompose in natural systems. As a consequence of these factors methods have been developed for the degradation and disposal of PCBs.

The present study examined the dechlorination of PCBs in marine sediment using electron beam technology. Aqueous surfactant was used to suspend the marine sediment (SRM 1944, New York/New Jersery Waterway Sediment) and to possibly enhance the degradation of the PCBs. Samples were irradiated at 50 kGy and 250 kGy. Following irradiation, each sample was filtered to isolate the sediment from the aqueous surfactant and each phase of each sample was examined for decachlorobiphenyl and biphenyl. Sediment sample preparations consisted of sample extraction using pressurized fluid extraction followed by clean-up with solid phase extraction. Aqueous surfactant sample preparations consisted of liquid-liquid partitioning with hexane and acetone followed by clean-up. Sample analysis consisted of gas chromatography and mass spectrometry. Results suggest that subjecting marine sediment-associated PCBs to a dose of 250 kGy completely dechlorinates sediment-associated decachlorobiphenyl. Concentrations of decachlorobiphenyl and biphenyl observed in the sediment and surfactant phases will be presented.

North Carolina State University

Improving the Performance of Point-of-Care and Bio-Warfare Detection Methods that Use Portable Fluorescence Spectrometers
Ryan Hill

Fluorescence spectrometric methods can be used for detection of clinical diagnostic and bio-warfare agent targets, such as glucose and anthrax. With an increasing demand for bio-agent detection, fluorescent standards need to be developed. This research project characterizes fluorescence detection using portable and benchtop fluorometers.

Portable fluorometers are increasingly being produced for point-of-care and in-field biological agent detection assays. These assays are designed to detect and quantify the amount of a particular target compound. It is important that fluorescent standards are developed to enable calibration of portable fluorometers with minimal effort and optimal accuracy.

In this project, the particular test target is a complex formed from dipicolinic acid (DPA), extracted from anthrax endospores, and terbium in solution. A comparison was done with both fluorometers to determine fluorescence intensities, characteristic wavelengths, and limits of detection of dipicolinic acid (DPA). Both fluorometers were calibrated using conventional and more user-friendly techniques. Results show a significant difference in the level of detection between the research-grade fluorometer versus the portable fluorometer. Correlations between the concentration of DPA, corresponding to the number of anthrax endospores, and fluorescence intensity were demonstrated.

Oregon State University

Development of Simulation of Job Shop Processes
Cary Maunder

Simulation is used to test new process plans, identify choke points in manufacturing flow, and optimize plant productivity in much less time and at a greatly reduced price than a manual reconfiguration. For most small job shops, however, it costs more to make a meaningful simulation of a process than the benefits warrant. Currently, there is not any commercial software that provides accurate pre-defined models for shop simulation, nor is there any standard interface for converting shop data into simulation data.

The NIST Manufacturing Simulation and Modeling Group has developed such a standard interface using a user-defined markup language called XML, which stands for Extendible Markup Language. They are now using commercially available software to develop turnkey models for job operations. Once the models are assembled, a process can be entered in XML and the simulation of the process can begin with minimal setup.

This presentation will outline the modeling process of a machine shop, explain what the next steps are for interfacing the model with XML, and show in some part manufacturing simulations to demonstrate the true power of simulation in process planning.

Pomona College

Spectroscopy of Er for Cooling and Trapping Purposes
Han Yong Ban

There has been recent success in the isolation of single Cr atoms using magneto-optical traps (MOTs) by the Electron Physics Group at NIST. The ability to control a single

atom has shown great potential for a vast range of applications in nanotechnology. In addition to Cr, Er appears to be an attractive candidate for single-atom isolation because of its high magnetic moment and its closed energy transition from the ground state $4f^{12}$ $6s^2$ $^3H_6$ to the $4f^{11}$ ($^4I^o_{15/2}$) $5d_{5/2}$ $6s^2$ $(15/2, 5/2)^o$ state near 841nm. This transition is within the range of commercial near-infrared diode lasers. Trapping of Er using a MOT has never been previously done. To achieve this, locking the pump lasers to this particular energy transition is required. To study the possible locking schemes, the spectroscopy of Er vapor was obtained using optogalvanic signals from a hollow-cathode discharge (HCD) cell. Saturation absorption spectroscopy (SAS) was used to acquire Doppler-free optogalvanic spectra. This revealed a superposition of a Lorentzian curve along with a Gaussian background due to velocity-changing collisions (VCC). The VCC broadening posed a significant problem for laser-locking. Two possible approaches to the solution of this problem were taken involving the use of an acousto-optical modulator and a homemade HCD cell. Spectra results will be presented.

Princeton University

A Differential Equation Approach to the Determination of the DMA Transfer Function

Van John Molino

The aerosol industry produces more than 1500 different products that generate over 10 billion dollars in annual sales. As computer chips and other components continually decrease in size, smaller and smaller aerosol particles begin to interfere with the functioning of these parts. Consequently, the classifying and sizing of aerosol particles is of great interest. The Differential Mobility Analyzer (DMA) is a commonly used tool for this purpose.

The first step in sizing these aerosol particles is finding the transfer function, defined as the probability that a particle that enters through the DMA inlet slit will exit via a sampling slit. This transfer function can be found by solving a stochastic differential equation. This process results in a second order linear partial differential equation.

Analytic solutions to the resulting partial differential equation can be found. The solutions are based on Bessel functions and the hyperbolic sine function. The transfer function can then be written in terms of an eigen function expansion.

This presentation will give a brief explanation of the DMA and its uses, but will focus on the mathematical aspects of this problem. The method for finding the analytic solutions to this differential equation will be shown and some of the complications that arise when working with the transfer function will be discussed.

Reed College

Structure, Chemistry, and Dielectric Properties of $Ba_3MgSb_xNb_{2-x}O_9$ and $Ba_3NiSb_xNb_{2-x}O_9$ Ceramics

Elizabeth Hopkins

Dielectric resonators make possible the widespread use of wireless technology including cellular telephones and base stations. Commercially used ceramics for wireless communications have the properties of high Q (low dielectric loss), high ε (allows for miniaturization), and low temperature dependence. The dielectric properties and composition of these ceramics exert an effect on the final size and price of the end products. $Ba_3ZnTa_2O_9$ and $Ba_3MgTa_2O_9$ are commercially used ceramics with excellent dielectric properties. The relative scarceness and expense of Ta_2O_5 led to substitution of Nb_2O_5 in previous studies. The dielectric constants (ε) of the niobium-based ceramics were larger, however also contained a larger temperature dependence and dielectric loss.

The systems $Ba_3MgSb_xNb_{2-x}O_9$ and $Ba_3NiSb_xNb_{2-x}O_9$ were investigated to determine the structural and dielectric property influence of a non-d^0 cation substituted for Nb^{5+}. The introduction of Sb^{5+}, a d^{10} cation, to the niobium crystal lattice site causes structural changes that may affect the dielectric properties of known niobium-containing systems. For a range of x-values, each new compound was synthesized, pelletized, and sintered to ~85-95% theoretical density. Their phases were determined from X-ray diffraction techniques, allowing the solid solution range for each system to be defined. The dielectric properties of these compounds were measured at microwave frequencies at TCI Ceramics, Inc. A preliminary analysis of the dielectric properties and the relationship to the phases will be presented.

Rensselaer Polytechnic Institute

Optical Tweezers Tip-Tilt Mirror Analysis

John Lippiatt

Currently there is no instrument capable of assembly of nanometer scale components. Optical tweezers is a technique that has been proposed to perform this task. Optical tweezers have the ability to trap and manipulate small spheres and rods with laser light. Here at NIST an advanced optical tweezers apparatus is being built for manipulation of nano-particles.

In controlling the optical tweezers an intuitive interface is desirable. A haptic device has been chosen to control the trapping beam and is in the process of being interfaced

with the beam steering optics and a vision system. Various issues with this interface will be discussed.

In the optical tweezers experiment a tip-tilt scanning mirror is used to steer the trapping beam. This poses a potentially serious problem: steering a beam in two dimensions with one mirror produces scanning nonlinearities. These nonlinearities produce curved scan lines when the mirror is offset in one axis then dithered in the other axis. This is particularly undesirable when trying to trap a straight rod where a curved scan line will not be sufficient. A Mathematica model of the system, which is used to correct for this and other errors, will be presented.

The Use of Real-Time Polymerase Chain Reaction in Quantifying Inflammatory Responses to Biomaterials

Sherry Lippiatt

The application and importance of synthetic materials (biomaterials) is expressed by the introduction of tissue engineering methods for the repair and replacement of human body components. Implanted biomaterials frequently evoke inflammatory responses, and are subsequently responsible for implant failure. We have established a system that allows for the analysis and quantitation of cellular inflammatory responses *in vitro*. Elevated cytokine production serves as an indicator of inflammatory responses, thus we monitored the levels of interlukin-1β produced by the cells. In this study, the inflammatory responses of non-transformed murine macrophages (Raw 264.7) cells were analyzed after incubation with polymethylmethacrylate (PMMA) microspheres in the presence and absence of lipopolysaccharide (LPS) at 18 hrs. The analysis of the genetic material obtained from the macrophages was quantitated using Real-Time Polymerase Chain Reaction (RT-PCR). RT-PCR can be used to rapidly and quantitatively analyze several gene products from multiple small samples simultaneously. Additional techniques utilized to quantitate the viability of the cells were flow cytometry and florescence microscopy. The goals of this work are to develop improved measurement methods for the quantification of cellular inflammatory responses to biomaterials and to obtain data that culminates in an enhanced understanding of the ways in which the body responds to the introduction of biomaterials.

Towards Attofarad (10^{-18}F) Capacitance Measurements: A Comparison of Capacitance Sensor Designs

Mark Matarazzo

As critical integrated circuit (IC) dimensions become smaller, high-resolution microscopy techniques grow increasingly necessary. Scanning Capacitance Microscopy (SCM) measures the capacitance between the probe tip of an Atomic Force Microscope (AFM) and the sample as the tip is passed over the surface. The resolution of SCM

measurement images is therefore limited by tip size, system noise, and system sensitivity. In this project three sensors based on the traditional L-C-R resonant circuit system and one sensor using a novel 180-degree phase shifting "bucking circuit" were explored. Analysis was aided by the use of a custom-built testbed with capacitance values ranging from 125 to 250 femtofarads. The sensitivity of each sensor was then measured and results were compared to determine the best system.

Rhodes College

Selective Electro-deposition of Actinides

Dustin Diez

When studying environmental radiation it is necessary to be able to separate actinides of different radioactive elements from a single sample. Currently, the most used procedure for separating out actinides is chemical separation. Those who are especially interested in spectroscopy rely on good separation with little contamination to maximize their signal. With chemical separation good separation of the actinides only occurs with perfect chemistry. This entire procedure can take up to several weeks. Once the samples are separated they can be electro chemically attached to a plate for spectral counting. If the chemistry was not performed to near perfection the spectra will not be reliable and the procedure must be redone. Because of the tedious time consuming nature of the separation chemistry it is important that we search for better methods to separate radio actinides. For example, if there exists a method in which one could selectively electro-deposit these actinides all the separation chemistry would become unnecessary. This would be a time saving procedure that uses minimal chemistry to achieve separations that will give maximum signal.

The goal of this experiment is to empirically determine if it is possible to selectively electroplate the radio actinides from a solution that has not been chemically separated. Currently, the exact mechanism for deposition of these actinides is unknown. If the mechanism of deposition is precipitation as a result of a localized PH near the cathode due to hydrogen evolution then selective deposition will not be possible. But, if there exists an actual charge transfer reaction where the oxidation state of the actinide changes near the electrode then there should be a thermodynamically derived reversible potential. This would be the basis for a selective deposition procedure of actinides. This experiment is performed by controlling the potential across a cell. The potential is measured against a standard reference electrode so that we are not measuring just the cell potential. This procedure will determine at what potential the actinides will separate and the order in which they must be deposited.

Rochester Institute of Technology

Properties of Polymersomes: A Practical Use of the Optical Tweezers and Scalpel

Lara Crigger

In the rapidly emerging field of biotechnology, scientists are continually searching for new methods of optimizing drug transport, delivery, and reactions. One such technology is the development of diblock copolymer vesicles, or polymersomes. Although they are amphilic like their lipid-based counterparts, polymersomes are distinguished by their increased durability and stability. These vesicles potentially could be used as nanovials for small-scale reactions; before this can happen, however, it is first helpful to fully understand their biomechanical properties and capabilities.

In this presentation, the author will discuss several experiments carried out this summer to investigate polymersome properties; the talk will begin with a brief review of the research done thus far on the subject. The physics behind such tools as the optical scalpel and tweezers will be examined in detail. Following will be an outline of the experiments conducted, including attempts at cross-linking the polymersomes for increased rigidity and an investigation of osmotic pressure as a driving force in membrane peeling and fusion. Pertinent results will be summarized, and possibilities for further research in this field will be considered.

Saint Joseph's University

Prostate Cancer Seed Calibration and Characterization

Joshua Scheuermann

Every year 1.2 million Americans are diagnosed with cancer, but the U.S. cancer mortality rate has decreased by 0.8 percent on average each year since 1990. This is due to the many advancements in cancer treatment. One such treatment is brachytherapy, a form of radiation therapy that delivers the radiation dose from sources within the body.

This summer I was directly involved in the calibration and characterization of radioactive, brachytherapy sources, called seeds because of their shape and size, used to treat prostate cancer. NIST maintains the national standard for the calibration of prostate cancer sources, and manufacturers are required to send seeds to NIST each year for calibration. A calibration involves a measurement to verify the strength of the seed, but also various other measurements used to characterize the different seed designs. Together, all of these measurements allow the researcher to observe differences between sets of seeds that the manufacturers send, as a method of quality control. This summer a new technique was developed to obtain a magnified, highly

resolved image of the radiation output of the seeds, allowing the researcher to see the actual distribution of the radioactive material inside of the seeds. Using a pinhole aperture, the seed is placed above the aperture, and a Fuji film Imaging Plate below the aperture, creating a Pinhole Camera. The distances of the seed and the plate from the aperture determine the magnification of the seed. This method of seed characterization could allow the researcher to see differences in radioactive distribution that could hint at changes, either intentional or unintentional, in the manufacturing process.

Saint Mary's College of Maryland

Flame Size vs. Heat Release Rates
Ian Rafferty

The heat release rate of a burning polymer is useful for assessing material flammability. It is also a fundamental parameter used to describe the growth and spread of large fires. Existing methods of measuring heat release are effective and accurate but require relatively large samples, expensive equipment, and are time consuming. The goal the present research is to create a faster, cheaper method that could be more widely used.

A current widespread method for measuring heat release is based on the cone-calorimeter, which determines the heat release rate from the burning sample by measuring the oxygen consumption rate of the flame. Since existing theory predicts that oxygen consumption is proportional to flame area, the flame area could be used to determine heat release. Our approach is to design a burner with small, geometrically stable, laminar flames, for which the oxygen transport is by binary diffusion. An optical system captures the flame image and digital image processing techniques provide the flame area. For flames of gaseous fuels, the correlation between flame area and heat release is excellent; for solid and liquid fuels, we are working to improve the correlation.

Santa Monica College

CMOS MEMS Test Structures for the Measurement of Young's Modulus
Peyman Kangavari

As the semiconductor industry further advances CMOS technology, by reducing the size of the transistors in integrated circuits (IC's), the interconnects, or wires that connect the transistors together, are becoming more complex. For instance, the process now used by Intel to manufacture their microprocessors may have seven or more layers of interconnects. One of the concerns associated with the development of complex interconnect systems is stress-related failures due to mechanisms such as

electromigration, stress migration, and delamination that are attributed to increased residual stresses in the interconnects.

The purpose of this project is to develop methods to characterize the residual stress in each layer of the thin-films in a VLSI process using CMOS-compatible, MEMS-based, multilayer cantilever test structures. In our approach, the residual stress is not measured directly; instead, measurement of the residual strain and elastic modulus are used to determine the residual stress. Our effort was to demonstrate the feasibility of measuring the elastic modulus using the resonant frequencies of cantilever beams. To achieve this goal, thickness test structures and cantilevers were fabricated through a commercial CMOS process. The thickness of each layer was measured using an optical profilometer on the thickness test structures. The resonant frequencies were measured using a laser Doppler vibrometer on the cantilever test structures. Finally, a model was developed to extract the elastic modulus from the measured thickness and resonant frequencies.

Methodologies for Measurement of TiO_2 Photoreactivity
Therasa Kim

Titanium Dioxide (TiO_2) is used as a filler for polymeric materials and is also a metal oxide semiconductor with photocatalytic properties that can facilitate decomposition of harmful substances on surfaces, and in air and water supplies. However, this same property can contribute to the degradation of materials in which TiO_2 is contained, such as coatings, plastics, and paper. In both cases, a need exists to accurately measure and characterize material properties of TiO_2, which contribute to its photoreactivity.

Although there are many different methods of measurement used in industry to measure photoreactivity, no scientifically-based, universal method exists. This portion of the project consisted of optimizing fabrication of TiO_2 specimens for photoconductivity tests by investigating various methods of specimen preparation and carrying out photoconductivity tests on selected TiO_2 samples while investigating the influence of external variables such as temperature, humidity, voltage, and UV intensity. In addition, series of TiO_2 samples were inspected through confocal microscopy in order to investigate the effects of film thickness and structure.

Concrete Microstructure and Aggregate Shape on the Millimeter Scale
Ji-Young Shin

Many of the macroscopic properties of concretes and mortars can be traced to the microstructure and topology on the millimeter scale. This microstructure in composed of inclusions (i.e. aggregates) of variable sizes randomly dispersed throughout a bulk matrix (cement paste), as well as a third feature known as the Interfacial Transition Zone (ITZ) of statistically greater porosity surrounding the inclusions. Based on

percolation theory, the topology of the interconnected ITZs with varying thickness and within different composites has been modeled by the Hard-Core/Soft-Shell (HCSS) modeling program to describe certain transport properties.

In addition to ITZ topography and varying aggregate size distribution and volume fractions, the properties of concretes and mortars also depend upon the 3-dimensional shape of the inclusions. 3-D real images of samples acquired by x-ray tomography can be analyzed using spherical harmonic functions, then used to generate VRML images. A database of aggregate shape images can then be used to classify aggregates from different sources, to correlate performance properties with actual surfaces and geometries, and for use in modeling programs such as HCSS.

Southern Methodist University

Autonomic Service Registration for the Service Location Protocol

Mackenzie Britton

Distributed systems require strategies to detect failures. Many systems employ a two-way heartbeat algorithm, where clients periodically probe servers, which respond to each probe. A missing probe suggests client failure, while a missing response suggests server failure. Faster heart rates mean lower failure-detection latencies, but also consume more resources. For a given heart rate, resource use also increases linearly with the number of clients. In this talk, I'll describe and characterize an autonomic algorithm that continually measures system size and adjusts heart rates within a defined range to bound resource use, while providing the best failure-detection latency for available resources and system size. The algorithm also constrains system capacity to guarantee worst-case average failure-detection latency. We apply the algorithm to regulate service registration in the Service Location Protocol (SLP). Specifically, we modified SLP service-registration procedures so that each SLP server returns a refresh rate to each client registering or refreshing service descriptions cached at the server. This feedback loop permits SLP servers to modulate the rate of client contact. Using these procedures, SLP servers constrain resource use and bound failure-detection latency, while providing the lowest available average failure-detection latency as the number of clients varies. We implemented our autonomic service-registration algorithm in a SLP simulator and conducted controlled experiments repeatedly adding and removing clients, while measuring client population, resource consumption, refresh rate, and failure-detection latency. Our simulation results yield close correspondence to predictions from an analytical model of our autonomic heart-rate algorithm. We discuss future work to implement our algorithm in a publicly available implementation of SLP, and then to conduct measurements and validate them against our simulation results and theoretical predictions. We also describe how our autonomic heart-rate algorithm

can be applied to regulate client-server query systems, subscription systems, and leasing systems.

Ferromagnetic Resonance in Thin Magnetic Films
Alan Skaggs

In order to store data on a disk drive, the magnetic moment of a few grains of the media must be switched. The speed at which the data can be written and read depends upon the ability to rapidly change the magnetization of these grains. When a bit of memory is accessed, it is "pinged," which causes the magnetization of the grains to oscillate. Damping mechanisms present in the film decrease the time needed for stabilization. Therefore, these damping effects play an important role in determining the speed at which the bit can be accessed. Some of the sources of damping are the absorption of energy by electrons in the metal, and the lattice vibrations. In order to provide optimum performance of the magnetic film for recording purposes, the main source of the damping must first be identified.

Ferromagnetic resonance (FMR) is a measure of the susceptibility of the film to an applied magnetic field. By measuring the microwave absorption of these films, important data can be obtained. The most useful characteristic for the application of FMR to storage media is the time required for the magnetization to "damp out," which is measured as the resonance line width of the sample. Since the line width is a function of both the damping and the defects of the material, it is important to separate the effects of defects.

The films used in this experiment all consist of the ferromagnetic material $Ni_{80}Fe_{20}$ (Py) deposited between layers of non-magnetic Ag. Since Ag and Py are immiscible, Ag goes into the grain boundaries, separating the Py grains and allowing them to behave with fewer interactions from neighboring grains. For thicker films, it is known that dipole-dipole coupling among grains increases. To observe the effects this has on the FMR spectra, three different film samples were tested, having thicknesses of 20, 100, and 200 angstroms of Py, but otherwise identical chemical composition, and subjected to heat treatment between 260°C and 300°C.

State University of New York – Binghamton

Mapping eBusiness Specifications
Shi Zhi Chen

As we know, e-Commerce has become increasingly important in today's business world, especially within the electronic and semiconductor industries. Unfortunately, there is not a single e-Business standard when transferring business documents

between sellers and buyers. As we can imagine, existing multiple standards result in lots of incompatibility issues when companies using different standards want to communicate with each other. That is the driving force to develop mapping transformations between major e-Business standards.

Our project's goal is to demonstrate the feasibility of using transformation between different standards. This is to ensure that companies can communicate with each other with reduced difficulty. The success of this project will have a great impact on global e-Business and economics within the electronics and semiconductor industries.

This summer, I have worked on the mapping between two major standards, RosettaNet Partner Interface Process (PIP) and OAGIS's Business Object Documents (BOD). The mapping was done from element to element. The different structure of these two standards causes the major difficulty during the mapping. In addition to the mapping, I also wrote an XSLT program to simulate the transformation.

Tougaloo College

RoboCrane: Advancement in Construction Site Technologies

Julius Rainey, Jr.

As the population of the world continues to grow at a quick rate, more buildings are needed to accommodate the many businesses of the world that are essential to the people. However, current construction sites consist of manually operated machinery, which can make the process of construction very slow. In addition, each year thousands of workers in the construction industry are injured or even killed.

With the desire to improve the project delivery time, the costs of constructing steel buildings and reducing the number of worker injuries and deaths on the construction work site, the Construction Metrology and Automation Group (CMAG) of the Building Fire and Research Laboratory Division (BFRL) is currently working with RoboCrane, an automated crane based on an inverted Stewart platform design that can pick and place beams.

In order for RoboCrane to know the position and orientation of the steel beam relative to a beam holder, research is being conducted into using vision software created by the Intelligent Systems Division (ISD). This software is an edge detection program that currently uses a web cam to determine the boundaries of a road so that autonomous driving can take place.

This presentation will include a description of RoboCrane, why it is important, and how CMAG is planning on using the vision software with RoboCrane.

Tulane University

Systematic Studies in the emiT Time Reversal Violation Experiment
Leah Broussard

The emiT experiment tests time reversal symmetry in the beta decay of polarized free neutrons by precisely measuring the T-odd triple correlation $\sigma_n \bullet \mathbf{p}_e \times \mathbf{p}_\upsilon$, where σ and $\mathbf{p}$ represent the neutron spin and decay product momenta, respectively. The experiment is in the process of acquiring data from its second run, which should ultimately produce a new limit on the D coefficient of approximately 2×10^{-4}. This result would significantly improve the current limit, an important step in further constraining extensions to the Standard Model. A preliminary analysis of some of the systematic effects in the data will be presented. These effects include timing information, such as the proton-beta detector correlations, and the observed spin asymmetry and its dependence on the beta energy. The gradual shifts of the proton energy peak and the effects of certain changes in system status on the spectra will also be discussed. The results of this data provide a qualitative analysis of the performance of the apparatus.

Radiative Decay of the Neutron
Alexander Wiener

Free neutrons decay radiatively roughly 1.5% of the time, emitting a proton, and electron, an antineutrino and a photon. While predicted, this decay mode has never been measured. The Neutron Interactions and Dosimetry Group is building an apparatus to detect the triple coincidence of a proton, an electron, and a photon from neutron decay. At present, various detection aspects are being investigated. The Monte Carlo N-particle Transport Code (MCNP) has been used to simulate electron and photon detection. With this tool, energy spectra have been simulated, which can later be compared with experimental data to assess the electron and photon detectors. In addition, two charged particle reamplifiers have been tested and compared to determine which would yield less noise and hence better measurements for electron/proton detection.

University of California – Berkeley

Planning on Traffic Growth in Optical Access Networks
Liliya Krivulina

The introduction of new high bandwidth services such as video-on-demand by cable operators will put a strain on existing resources. It is important for cable operators to know how many resources to commit to the network to satisfy customer demands. We developed models of voice and video traffic to determine the effect on demand growth

on hybrid fiber-coax networks. We obtained a set of guidelines that network operators can use to build out their networks in response to increased demand. In the course of the research, we looked at different types of data that could be sent over a network and amounts of bandwidth associated with that. We primarily concentrated our attention on such services as downloading and video-on-demand systems since they seem to be widely used when high-speed connections are involved and appear to be popular nowadays. Initially, we started out with only one type of traffic and later added another type to obtain probabilities of network loads. Such estimations helped us determine how networks would function under various conditions (i.e. low, medium, and heavy loads). Also, we took into consideration how the growth rate of the popularity of such services would change over time. Our finding will help cable operators estimate how much bandwidth they need to provide to a given level of demand.

Interferometry: PSI and VSI Discrepancies
Jonathan Lee

Interferometry is a powerful form of optical microscopy. Interferometric microscopes measure samples in three dimensions, down to the nano-scale in the vertical direction. Interferometry works by sending a light beam down to a sample surface, and its reflection beam combines with a reference beam. When the two light waves propagate together, interference patterns can be analyzed to determine the contours of the sample's surface. At NIST, we have a microscope called WYKO NT2000 that measures with two modes: Phase-Shifting Interferometry (PSI) and Vertical-Scanning Interferometry (VSI). PSI measures in a range from 1 nanometer (nm) to 160 nm while VSI measures from 3 nm up to a few millimeters. Intuitively, we would expect the two modes to agree on measurements in the measuring range from 3 nm to 160 nm. However, before the summer, a discrepancy between the two modes was observed.

I was assigned to investigate this discrepancy. The approach was to verify the reliability of the microscope's hardware and software. My focus for a good portion of the summer was software testing. C++ programs were written to simulate datasets with unique patterns and to recreate the data analysis. WYKO's output data and analysis could then be compared with simulated datasets and known analysis algorithms.

This talk briefs the concept of interferometry, the differences between PSI and VSI, and the WYKO software. It also describes data collected and the methods used for examining the software. Finally, it identifies findings and recommendations.

Integration of Microcontroller for Embedded Gas Sensor System-on-a-Chip
Iris Wong

Today, portable devices for detecting toxic airborne chemicals are largely limited to specialized equipment designed for use by the military or by first responders to

chemical spills. Current trends in chemical sensing suggest that a smart, small, and low-cost integrated sensor system is highly demanded to serve as an early warning system for the presence of environmental pollutants, chemical warfare agents, and trace explosive detection.

NIST is currently conducting research on a class of microsensors, which uses an array of MEMS-based CMOS-compatible microhotplates with post process deposited metal-oxide sensing films. A key advantage of this technology is that an array of microhotplates with various types of films can be programmed to cycle through specific temperatures. If a specific chemical of interest is present, the conductance of the sensing film produces a "signature" that can be matched against a library of chemical signatures to identify both the type and concentration of the gas in the ambient air.

To enable rapid and cost-effective deployment of the gas sensor technology, System-on-a-Chip (SoC) integration with logic, memory and analog circuitry is necessary. To do this, the gas sensor must be represented as a Virtual-Component (VC) that is compatible with the existing digital SoC design methodology. The gas sensor VC must include a digital interface and be compatible with the Design-for-Test (DFT) protocols used for SoC design. The NIST gas sensor VC consists of an array of microhotplates with individually programmable heater power amplifiers, and a multiplexed Digital-to-Analog-Converter (DAC) that measures the sensor film conductance and temperature sensor voltage.

It is the purpose of this SURF project to integrate and program a microcontroller to control and monitor the signals necessary for gas sensing functions. An MSP430 microcontroller system development board is used as a test vehicle for the initial interfacing and programming. The developed microcontroller algorithms generate and control the heater power waveforms, monitor and decode the temperature sensor voltage and sensor film conductance waveforms, and provides appropriate responses to interrupts. The hardware interfaces and control algorithms developed will form the basis for development of the gas sensor VC interface and the future monolithic integration of the gas sensor SoC.

University of California – Irvine

A New IMPACT in Silicon Carbide Power MOSFETs
Tam Hoang Duong

Power semiconductor devices are the key enabling technology for high frequency power switching conversion applications. The Insulated Gate Bipolar Transistor (IGBT) is the dominant power device used for medium power conversion applications from 1 A, 600 V to 1 kA, 6.5 kV with annual sales of about $1B. The medium power conversion applications market is about $40B annually and includes applications such as automotive ignition systems, industrial motor drives, electronic lighting ballasts, and traction motor drives from electric vehicles to diesel-electric locomotives. Emerging power device technologies that utilize the SiC material promise to extend high frequency power conversion into the 10 kV to 25 kV range with applications in power distribution, energy storage devices, and ship propulsion systems.

In order for power conversion system designers to fully utilize the advantages of power devices, models are needed in system simulators and model parameter extraction tools are required to characterize commercial power device products. The defacto standard model used for the IGBT was developed at NIST by Hefner and resulted in $18 million benefit in reduced cost of designing products and $40 million annual benefit in product improvements largely due to energy reduction. NIST also introduced the IMPACT (IGBT Model Parameter ExtrACtion Tool) software for extracting parameters for the IGBT models. NIST researchers recently also developed SiC power device models and extended IMPACT to include SiC MOSFETs.

The objective of this SURF research project is to provide the software tools necessary to extract the model parameters for the most recent version of the IGBT and SiC power MOSFET models. A new extraction algorithm and automated measurement system is developed to characterize the gate and gate-drain charge characteristics including the effects of negative gate voltage inversion of the gate-drain overlap region. The new extraction procedure enables the extraction of the gate-drain overlap inversion threshold voltage and gate-drain overlap area. The new software is demonstrated by extracting parameters for the first time for an advanced high power full-bridge IGBT module and a first-of-a-kind SiC power MOSFET.

Binary Analysis of High Volume Data Sets
Adaeze Esiobu

The National Software Reference Library (NSRL) is designed to collect software from various sources and incorporate file profiles computed from this software into a Reference Data Set (RDS) of information. The Reference Data Set can be used to uniquely identify files on a computer by law enforcement, government and industry.

Law enforcement uses this Reference data Set to determine what files are necessary for evidence on a seized system.

Often software exists in more than one language version in order to accommodate global usage. Because the NSRL project must uniquely identify each file (and each version of each file) it must have a specific entry in its RDS for each language version. The addition of all of these entries into the library costs a lot of money and time. Throughout this summer we worked on trying to determine one of two things:

1. Is each language version totally unique thus requiring acquisition/processing of all language versions?
2. Is there a matching pattern that can be identified and utilized to define the common parts between all language versions of a file that change or do not change?

We did this by comparing binary file contents of different language versions for the same software and tried to see if they only differed in the language specific part of the software and nowhere else or otherwise. Through binary analysis we sought to either rule out any case of similarities between both language versions or assert the similarities between the versions except in language specific areas. Much of this analysis was done on large data sets. One of the main goals of being able to answer the question at hand is to find ways of optimizing the performance of the NSRL therefore saving money and time. As a result of this, the National Software Reference Library up till date has had to keep track of every language version of software and it's Reference Data Set of Information and this could get really expensive and time consuming if it was necessary for the National Software Reference Library to acquire every language version of software or if one language version of software will provide sufficient information for all other language versions of the software that might exist.

Verifying and Standardizing Functionality of Forensic Hardware Devices

Akash Garg

Law enforcement officials analyze evidence captured from criminal investigations of various natures. A wide variety of prominent evidence lies on hardware storage devices. Consequently, officials require a method of accessing this underlying data on storage devices and analyzing it so that it can be used as evidence in the court of law. However, digital data is vulnerable to modification by either human error or by unlawful action. Such modified digital evidence would then be disregarded in the court of law, as there is no guarantee to its integrity. Therefore, several methods have been developed with dual goals of protecting data from modification as well as allowing one to extract and analyze the protected data. Four of the most common data protection methods developed by computer investigators are: (1) operating system based protection allowing protection and extraction in read-only mode (2) BIOS (Int 0x13)

based software write protection (3) direct access/driver based software write protection and (4) hardware based write protection using hardware write blockers. Each of these techniques has particular advantages and disadvantages. Nevertheless, the most effective and reliable method is generally accepted to be data protection via hardware write blockers. As a result, computer investigators rely heavily on hardware write blockers as a means of data protection on storage devices, while accessing data for analysis. Although these devices play an important role in computer related criminal investigations, they have not yet been held accountable to a common standard of functionality. This lack of a functional standard has effectively reduced the credibility of evidence obtained from such devices. Our research fills this void by developing a specification and methodology for verifying that such tools comply with standard functionality.

"In Search of a Hot Pig" – Thermal Detection of Radioactive Materials

May Liang

Radioactive dispersal devices spread radioactive materials through explosions. The radioactive materials that maybe used are readily available for medical or commercial uses. They may even be gathered from foreign countries and delivered to the U.S. under the disguise of legal cargo. To prevent nuclear terrorism, it is ideal to adopt an efficient method of detecting these hazardous materials before it reaches the public. Once the radioactive material is shielded in a lead container, the detectability of the radioactive materials by conventional scintillator decreases. Thermal imaging is an alternative technology to be explored.

Using heat sources to mimic the heat generated by a Co-60 source, experiments were done in two separate lead containers. The objective is to explore the nature of the remote sensor, by varying the power of the heat source, and observing the temperature difference over time. The digital imager consists of an array of superconducting InSb photo diodes, capable of sensing thermal differences of 0.05°C. The calibrated data is first converted into the correct format through LabVIEW, then analyzed using ORIGIN. Ultimately, the detection limit of the remote sensor will be the crucial point in arguing the feasibility of this thermal detection method.

Although the data from an infrared camera might not be sufficient evidence, when use in conjunction with an x-ray machine and a scintillator, the probability of a false alarm is lessened.

Temperature Control in the Molecular Measuring Machine
Alice Nguyen

To assist Nanotechnology in its thriving developments, the Molecular Measuring Machine (M^3) provides precise measurements and images of surface features for various samples. The two-dimensional coordinate measurements that M^3 produces are to be within nanometer uncertainties over a 50mm by 50 mm area.

To achieve such accuracy, any possible environmental disturbance is damped by an assortment of control systems. Temperature control of the M^3 is necessary in order to maintain a low measurement uncertainty. If the temperature were allowed to fluctuate, the measurements would be subject to significant error at a molecular length scale. Therefore, the core of M^3 is made from a solid copper sphere because of copper's high thermal conductivity, which will minimize the temperature gradients, allowing the temperature to distribute uniformly. The core is heated by radiation from a heater shell and cooled by the environment surrounding it, which is kept at a temperature about 3° lower than the target temperature of 20°C. The temperature control is able to maintain temperatures within 5 millidegrees. This summer I upgraded a program from Basic to LabVIEW in which the computer interfaces with a voltmeter, scanner, and multimeter. The multimeter measures the resistance of 5 platinum resistance thermometers and the voltmeter measures the voltage of 18 thermocouples. These resistances and voltages are then converted into temperature within the LabVIEW program, and controlled by a PID controller. This will allow careful monitoring and elimination of any temperature fluctuations within the M^3.

A Method to Achieve CD Reference Materials with 100 nm Linewidths
Ravi Patel

As microelectronic devices shrink in size, due to performance and cost pressures, there is a need to be able to accurately manufacture their features having minimum dimensions. Line-width control is important to enhance performance as well as to reduce the size of devices. There are many different measurement techniques but the Scanning Electron Microscope (SEM) metrology is the most efficient in terms of cost and accuracy. However, SEMs provide less and less accurate measurement data as device size and line widths are getting smaller. This is where the reference features developed by this project come into play. The main goal is to develop reference features with very high accuracy to aid the measurements made by SEMs, and other instruments, as device size is decreased.

During the summer, our goal was to reduce the line-widths of the reference materials from 300 nm to 100 nm or less. To accomplish this, a process was developed that involved using silicon-etching solutions. The method uses a sequence of anisotropic, isotropic, and finally an anisotropic etching process. The initial anisotropic etch had

already been performed during wafer lithography. The plan was to undercut the silicon using the isotropic etch because it is not lattice-plane orientation dependent and can reach areas where the anisotropic etch could not. Then, we use the anisotropic etch in order to straighten the walls of the line feature once again. The isotropic and anisotropic etch used to perform these two final etches were, respectively, a Hydrofluoric-Nitric-Acetic acid mix (HNA) and Tetramethylamonium Hydroxide (TMAH). The results and data obtained from the performed method will be presented and explained.

The Kinetics of Cluster Formation of Polyethylene Oxide in Water

Jamaal Sanders

Polyethylene Oxide (PEO), a water-soluble synthetic polymer, is used in many applications worldwide, such as to reduce drag in pipe flow, to stabilize colloidal suspensions, and as a biocompatible agent for application in drug delivery. Surprisingly, the behavior of this polymer in water is still widely debated. Aqueous solution of PEO forms aggregates in water, but whether these aggregates are an inherent property of PEO or not is the controversy. Knowing if PEO aggregation is an inherent property will further help its uses in industry as well as polymer science. We have used Dynamic Light Scattering (DLS) and Small-Angle Neutron Scattering (SANS) to investigate the clustering of PEO in pure double distilled and filtered de-ionized water. Using dynamic light scattering, we have noticed that filtering and raising the temperature of the solution affect the clustering of PEO. Filtering the solution breaks up the clusters, which are about the size of 1 micron, but after a couple of days the clusters reform in the solution. The temperature of the solution has an impact on the clustering size of PEO in H_2O. Increasing the temperature changes the size of clusters that are formed. We have also used SANS, which is a more direct method for determining "particle" size, to complement the DLS measurements. Our data shows clusters reforming days after filtration and that the temperature effect on PEO is reversible. Both of these observations support the hypothesis that cluster formation is an inherent property of PEO in water.

Depth Profiling of Polymeric Samples Using SF_5^+ Primary Ion Bombardment

Shalini Varghese

A major concern with many implanted biomaterials, such as artificial organs and drug delivery systems, is the potential for undesirable interactions with the human body, which correlate with biomaterial surface properties. For this reason, the development of surface analysis techniques has become vital to researchers in the biomedical field. Time of Flight Secondary Ion Mass Spectrometry (ToF SIMS) is such a technique that uses mass spectral analysis and imaging to provide an abundance of information about surfaces, including their composition, structure, orientation, and molecular distribution in space. However, a major limitation of this technique is that it only analyzes samples at a constant depth of 1-2 nanometers. Therefore, ToF SIMS needs to be developed into

a three-dimensional technique for use in depth profiling polymeric samples. Recent experiments have shown that cluster primary ions, such as SF_5^+ are particularly useful for depth profiling because of its unique ability to cause a high sputter yield and minimal damage to a surface, unlike atomic primary ions, as Cs^+. In this project, substrates made from poly(2-hydroxyethyl methacrylate) (pHEMA), a polymer commonly used in ophthalmic biomaterials, have been profiled alone, derivitized with trifluoroacetic anhydride (TFAA), functionalized with the amino acid, L-Lysine, and studied for their stability under extended SF_5^+ bombardment. TFAA reacts selectively with the hydroxyl group of pHEMA and attaches its C-F group to the polymer, changing its surface chemistry. Attachment of L-Lysine to pHEMA serves as a model for peptide attachment to surfaces. The goal is to determine whether depth profiling of these polymeric sammples will provide all of the information present on their surfaces. Along with ToF SIMS, profilometry, optical microscopy, and infrared spectroscopy have been used to obtain additional information about polymer surface chemistry.

Visualization and Segmentation of Objects Based on Riegl Data

Eric Zhang

The goal of our project is to collect and analyze data from ladar sensors on the HMMWV (High Mobility Multipurpose Wheeled Vehicle) to develop algorithms for autonomous driving. One of the sensors used in this project is called the Riegl scanning ladar, which is a very powerful sensor with very high resolution, big scanning range and angle.

This project not only has valuable practical applications in the field of military combat and information collecting but also serves as a new foundation for robotic technology and artificial intelligence. Although with today's ladar technology, our algorithm is not fully applicable yet, but by developing the algorithm ahead of time, we can assure compatibility and parallel growth with the ladar technology.

My project is focused on analysis of the Riegl data. I began by developing C++ programs, which transform raw Riegl data into displayable files. From the same input data file, I was able to display intensity, rgb-color, and point cloud images from front, top-down, and side viewpoints. My goal is to design algorithms to visualize and segment out a particular type of object from an image, which I chose to be cars. My method of segmentation was to set threshold on height of objects. I set the lower limit to be the Â½ meters above the surface plane of the road and attempted to set the upper limit as the height of normal cars with respect to the road. In this way, everything that is left within the two thresholds were likely to be cars. The size of each object within the threshold was then used to segment out the cars from other objects such as tree trunks or road signs. To obtain the surface plane, I displayed images in 3D form and selected an area of the road. Then I took a sample of the selected points and applied surface fitting algorithms using Matlab. The output was a best-fit surface to all the input

points. The last step was to select more sample points from other areas of the road, following the same procedure, to recursively update the surface function.

Although this project is far from finish, it had a good start. Similar algorithms can be used in recognizing other objects such as trees, people and buildings. The programs can also be expended to work for multiple successive images during a real time driving experiment in the future.

University of Colorado – Boulder

Characterization of LED Power Distributions

Jennifer Scheib

As light emitting diode (LED) application expands beyond traditional indicator lights to uses such as traffic signals, color displays, and even general illumination, it is critical that standards for both source characterization and photometric scale transfer be defined. The Optical Sensor group at NIST is addressing these issues by developing an LED screening process that will initially be used to characterize the beam source distributions, distance-illuminance relationships, and temperature sensitivities. Eventually the process will be used to collect standard LEDs to transfer the lumen scale. The focus of the SURF 2003 summer project was beam source characterization, and specifically, checking optical and mechanical axis alignment among all varieties of LEDs. This involved completing the development of a small-scale goniometer that allowed for azimuth and plane angle rotation of the LED and translation of the detector. LABView was used to create an automated control system for data acquisition (detector voltage, detector temperature, LED forward voltage, and LED current) over approximately a 3π spatial extent from the tip of the LED. Critical issues addressed during the course of the project were error reduction in mechanical axis alignment and distribution modeling.

University of Kentucky

Simulating Quantum Circuits at the Gate-Level: QCSim

Andrew Lane

As we make progress in quantum physics, the goal of producing a quantum computer looms closer. Decades may pass before quantum computers are in widespread use, but with the power such a system could wield, the future is very bright. However, due to the very nature of quantum mechanics, such a system would be quite fragile. Therefore, it is imperative to develop robust error correcting schemes that protect the integrity and fidelity of any quantum system.

Quantum systems can be simulated classically, but the memory required increases exponentially as the system grows. Last summer, a basic quantum simulator (QCSim) was developed in C++, which simulated a quantum circuit at the gate-level. I significantly improved the front-end of QCSim by implementing a quantum gate language that allows for the declaration of qubits by name, an initialization of the quantum state, and quantum gates and operations. We implemented specialized gates that simulated various quantum errors. I wrote circuit descriptions for quantum communication (BB84) and quantum error correction (Steane 7-qubit). We compared the efficiency of various error-correcting codes and schemes and simulated quantum communication.

University of Maryland – Baltimore County

Digital Rights Management
Aolat Abimbola Adedeji

Digital rights management (DRM) is the practice of trying to secure intellectual property rights of digital contents such as mp3s, e-books, and software that are transmitted through the Internet. Initial DRM methods failed to focus on essential DRM requirements such as interoperability and convenience. Currently a slew of organizations attempt to mesh technical, business and legal concerns into an acceptable, interoperable and open service. As a guide on this developing group, Gordon Lyon compiled and published a document titled *A Quick-Reference List of Organizations and Standards for Digital Rights Management* in March 2002. This project entails the update of the current activities and organizations working on digital rights management contained in that document and including a listing of commercial entities that offer a form of DRM for digital content; in particular to the health care area, such as Questra Smart Service Solution. This quick-reference list will serve as guide for maintaining interoperability and aiding in the formalization of de jure standards in cross-industry digital rights management.

Modeling Near-Interfacial Defects in High-k Dielectrics
Michael Powers

High-k dielectric materials, such as Hafnium Dioxide, are widely investigated to offer the possibility of enhancing conventional MOSFET (Metal Oxide Semiconductor Field Effect Transistor) technology. These materials are proposed to replace lower dielectric constant materials, such as Silicon Dioxide, as the gate insulator in conventional MOS processes.

Hafnium Dioxide and other high-k dielectrics generally have more electron traps near the channel-dielectric interface than Silicon Dioxide. Traps are created when

unsatisfied bonds create potential wells due to material defects. The presence of traps decreases the carrier mobility in the MOSFET channel and causes channel resistance to increase.

In this work charge-pumping is used at various ambient temperatures to determine the density of near-interface traps. Charge-pumping is the process of pulsing the channel from accumulation to inversion causing charge to gather and then disperse from the region. This results in a net substrate current when some electrons are trapped. The substrate current is proportional to the defect density over a certain energy range. By changing the temperature and pulse characteristics, specific energy ranges within the bandgap are selected. Data from these experiments is used to determine the energy distribution of traps for Silicon Dioxide and Hafnium Dioxide. These results are correlated with other measurements, such as carrier mobility.

Plasma Diagnostics for a Dual Frequency Plasma Source
Marcos Vicente

Developments in semiconductor technology during the past 50 years have made electronic devices smaller, faster, and more reliable. A key component in accomplishing this has been through the use of plasma etching reactors. One such plasma etching reactor design is the dual frequency plasma sources. This system contains a top and bottom electrode to which two different RF frequencies are applied. This is done in an attempt to independently control the plasma density and RF bias. The plasma density controls the semiconductor etching and the RF bias controls the energy of ions hitting the semiconductor surface, which in turn controls surface damage, and etching selectivity.

Many traditional diagnostics, such as the Langmuir probe, do not work well with more than a single rf frequency. One diagnostic, which should work well with the dual frequency plasma source, is the microwave interferometer. In this microwave interferometer method that is applied, electromagnetic waves are used as a probe into the plasma, which with the proper measuring devices can measure the index of refraction of the plasma. The index of refraction is useful as it is directly related to the electron density, which is one of the key plasma parameters. The diagnostic will be used to monitor the plasma production for a variety of plasma conditions such as pressure, flow rate, rf power, and rf frequencies. These are the components that we are looking for in hope to enhance the next generation of semiconductor processing.

VOIP Security
Thomas Walsh

Voice over Internet Protocol (VOIP) refers to the transmission of speech across data-style networks. In recent years there has been a move within the telecommunications industry to refurbish their telephone infrastructure by incorporating VOIP technology.

Many companies have followed suit, citing cost saving potential and network simplifications to justify the move to VOIP. However, numerous unresolved security and privacy issues remain in the VOIP architecture, and the amalgamation of data and voice networks makes the compromise of either subsection twice as egregious as before. Complicating matters is the time–urgent nature of VOIP, where delays as miniscule as 150 milliseconds can cause an unacceptable degradation in Quality of Service (QoS). This restriction means the structures and procedures typically employed to secure data networks, including firewalls, NAT routers, and encryption need to operate extremely fast, or risk making the call virtually unintelligible. The speed problem is especially vexing for crypto-engines, because they lack support for QoS and may therefore cause a starvation situation for VOIP packets while servicing larger data flows. In addition to the speed issues, the introduction of firewalls and NAT routers into a network complicates the use of both of the two competing protocols for call setup in VOIP (SIP and H.323). Such devices can block incoming calls as well as the call setup process itself. Solutions for these incompatibility issues include Application Level Gateways and Proxy Servers. In the end, safeguarding VOIP is a matter of adapting traditional data network security elements and procedures for the fast paced dynamic world of voice communications.

University of Maryland – College Park

Organic Monolayers on Silicon(111)

Kelly Anderson

In recent years, computer processor speed has doubled roughly every 18 months, according to Moore's "Law." To accommodate this speed transistors have become smaller and chips more dense. However, as these transistors get smaller and smaller, the insulating oxide layer gets thinner, giving rise to electron tunneling, thereby destroying the usefulness of the device. If progress in this field is to continue, a new way of making transistors must be found. One promising avenue for this is the use of organic molecules as the insulating layer.

As a first step in accessing the electronic properties of metal-molecule-silicon structures, my research this summer involved the attachment of various organic molecules to hydrogen-terminated silicon(111) surfaces to form chemisorbed monolayers. Relatively little is known about the attachment of organic molecules and their electronic properties. In order to properly interpret the electronic properties, compare with theoretical predictions, and compare different chemically tethered monolayers, thorough physical and chemical characterization of the monolayers is necessary. After synthesis of the monolayers, I used infrared spectroscopy, spectroscopic ellipsometry, and contact angle measurements to characterize the layers. My presentation will

include a discussion of my methods and results, and potential use of these monolayers in electronic devices.

Air-Ground Sensor Registration
Anthony Downs

With funding from the Army Research Laboratory (ARL) and DARPA, NIST is developing architectures and algorithms for completely autonomous vehicles. The research makes use of the NIST Highly Mobile Multi-Wheeled Vehicle (HMMWV) and an experimental unmanned vehicle (XUV) developed under the Army's Demo III program. The vehicles make use of data from the Global Positioning System (GPS) as well as from sensors on the vehicles. In order to have a back-up for GPS, another method of self-localization is needed. In my research, I am making use of combined data from a scanning ladar rangefinder on the ground vehicle and a ladar mounted on an aircraft that flies over the terrain being traversed.

The approach to find and update the position of the unmanned vehicle involves registering data from the two ladars. The method uses an adaptation of the Iterative Closest Point (ICP) algorithm to estimate the vehicle's position by registering a scan from the range sensor mounted on HMMWV with one obtained from the aircraft flying over the same terrain. Registration enables the vehicle's position to remain known even if only one of the sensors has GPS information. Registration over time (i.e., from sample to sample) enables position information to be maintained even when both sensors lose GPS contact.

The approach is being validated by conducting systematic experiments on complex real-world data. The approach failed originally, due to differences in resolution between ladar scans, but with modifications, will pass.

X-Ray Absorption Measurements of Water Loss in Curing Mortar Samples
Kiri Feldman

After concrete is mixed, the interaction between environmental conditions and the temperature and moisture dependent hydration reactions that take place impact its strength and durability. If concrete becomes too warm or lacks sufficient moisture, it may crack or fail to reach its maximum strength. Ensuring that concrete receives adequate moisture, added in the mix and applied to the top surface, is critical to maintaining public safety, optimizing service life, and reducing repair costs. Our experiments employed an x-ray absorption system to examine water movement in cement paste and mortar specimens during and after curing. Curing conditions included saturated curing for 1, 3, and 6 days, sealed curing, and exposed curing. This study used ASTM Type I and blended Portland cement pastes with 20% mass flyash substitution, mixed in a water-cementitious materials ratio (w/c_m) of 0.4. The x-ray

absorption system provided an indication of the specimen density by measuring the amount of x-ray energy passing through each specimen. Changes in x-ray absorption counts over time correspond to changes in density due to water movement. Mass measurements were used to assess bulk water gain and loss. This presentation discusses the experiment methodology and results from this preliminary investigation.

Modeling Smoke Detectors
Jessica Kratchman

Conventional smoke detectors have two basic operating modes: normal and alarm. Emergency responders thus have little information about the conditions of a fire other than one has occurred. By analyzing data from recent fire experiments and comparing it with measurements of smoke concentration and detector activations, characteristics of smoke detectors can be defined, and fire models can be verified. Based on fire growth these models will tell emergency responders not simply the presence of a fire but also the critical characteristics associated with heat and smoke. Once these models are verified smoke detectors will be able to have their signals converted to smoke concentrations, heat release rates, flashover conditions, and more. These conversions can be displayed in graphic form giving fire fighters and other emergency responders a more informed and precise plan of attack with reduced injury, loss of life and property damage.

Various types of smoke detectors were first calibrated, resulting in equations that convert the detector signal to laser smoke concentration. These equations are used to convert the smoke detector output from small room fire tests to laser smoke concentration. Next, the entry time delays and the exponential time constants were determined for the different types of detectors using signals obtained from step-exposure tests. Step-exposure tests gradually increase the smoke density by increasing flow rate. The next step was to compare these experimental values with the values produced by the JET Fire Dynamics Model.

A summary of the procedure established to calibrate the detectors and discussion on the optimization of the detector will be presented.

Studying Protein Sequences Using Bioinformatics
Shirin Mehraban

Bioinformatics is a field that combines biology and information technology to develop tools that have successfully identified genes and proteins that are important for medical and biotechnology applications. The last decade has seen an enormous increase in the number of biological sequences that must be analyzed for potential use. The principal non-experimental method for doing this is multiple sequence alignment. Here a set of

protein sequences with unknown properties is matched with a set of protein sequences whose properties are known.

This summer we implemented and tested an algorithm that offers a promising new approach to the problem of aligning long sequences. Our talk will discuss the elements of this algorithm, which is based on probability model of the alignment process. Like other currently used algorithms a proposed alignment is based on a total maximum score. Individual scores are based on the likelihood that an amino acid can be substituted for another. Our algorithm computes maximum scores by solving a linear programming problem. We have done some initial comparisons with current alignment methods and get good agreement for ranges of model parameters.

Sheet Metal Studies on Fe-base Alloys

Timothy Quarrick

Driven by the requirement to meet government regulations, the automobile industry is striving to make vehicles more fuel-efficient. One approach to meeting this goal is to reduce the overall vehicle weight, thus resulting in better gas mileage. As a significant fraction of the vehicle's weight is the conventional carbon steel sheet that is used in constructing the outer body, efforts have been focused on transitioning to lighter weight materials (*e.g.*, dual phase steels, high strength low alloy steels, aluminum alloys) in these applications. However, implementation of these lightweight alloys has been slow due to both a limited knowledge of material behavior and a lack of experience in the sheet forming process. By obtaining a better understanding of the material characteristics (e.g., strain limits, surface roughening) during biaxial stretching, these materials can be more readily utilized for complex stamped components. The initial phase of the project for the lightweight steel grades requires a baseline study using a low carbon 1010 steel. Samples were deformed to various in-plane strain levels under balanced biaxial conditions. Characterization techniques used to study the changes in microstructure included optical microscopy, scanning electron microscopy, X-ray diffraction, and surface profilometry. From these results, relationships between the effective strain levels, relative change in crystallographic orientation, and free surface roughening were developed. These results will be used to understand the formability behavior of the dual phase steels in this ongoing research project.

Performance and Cost Tradeoffs for Use of Omni-directional Vs. Unidirectional Regenerators in Optical Networks

Richard Su

Optical switches currently use unidirectional regenerators. Each of these regenerators is pre-assigned to a specific ingress-egress port pair. Evolving technology allows the regenerators to be omni-directional, which means that regenerators need not be pre-assigned directionally but can be assigned on demand for any pair of ingress-egress

ports. This new technology has the advantage that potentially much fewer regenerators need to be used for a certain connection-blocking requirement as compared to the existing technology with unidirectional regenerators. In this research, we develop models to evaluate the performance and cost tradeoffs of these two technologies. In theory, current technology with unidirectional regenerators has the tendency to use up all the regenerators in one direction while regenerators in other directions are left unoccupied. Using unidirectional regenerators therefore leads to a waste of resources, but this can be resolved using the technology of omni-directional regenerators. The models we develop produce results that back up this theory under both normal and bursty network traffic condition. Additionally, the significance of using omni-directional regenerators for cost savings becomes more obvious as the network traffic gets heavier.

Testing for the Common Intersection Point of Lines
Chiu Yeung

The goal of this project is to develop a statistical test of the hypothesis that a collection of straight lines has a common intersection point, and credible estimators for the point and associated errors. This problem appears in multiple applications. In particular, at NIST and University of Maryland in a study of the so-called isokinetic relationship. Describing the empirical dependence between enthalpies and entropies in a series of related reactions among polychlorinated phenyls.

To derive an appropriate likelihood ratio test, the problem of finding the maximum likelihood estimator of the intersection point has been investigated. This problem involves optimization of a non-convex function, which typically requires a good initial approximation. In the balanced case, the estimator obtained from errors-in-variables methodology can be used as such an approximation. It is shown that the likelihood ratio test with F-distribution critical point is conservative, and that it can be derived from the intersection union principle. Monte Carlo results and an application of the test to real-life data are also reported.

Development of a Bismuth Filter for Neutron Vibration Spectroscopy
Ramsey Zeitoun

The neutron is a novel and powerful probe of condensed matter. It possesses no charge and interacts with atoms via nuclear rather than electrical forces, thus allowing it to penetrate through most materials. The wavelike properties of the neutron permits one to utilize diffraction methods to create beams of monoenergetic neutrons for use in such scattering techniques as neutron vibrational spectroscopy (NVS). NVS is analogous to photon-based vibrational spectroscopies such as infrared or Raman spectroscopy, but possesses unique properties that render it complementary to these spectroscopies and invaluable for probing the vibrational spectra of solid-state materials. One limitation of

the Filter-Analyzer Neutron Spectrometer (FANS), the world-class NVS instrument at the NIST Center for Neutron Research (NCNR), is the presence of spurious low-level background scattering from the beryllium (Be) filter used in the scattered-neutron analyzer. Such spurious scattering complicates the clean measurement of the vibrational density of states of more weakly scattering samples. It has been determined that this spurious scattering can be eliminated by an additional "polycrystalline" bismuth (Bi) filter placed in front of the Be filter. The development of a Bi filter with sufficient polycrystallinity is nontrivial since bismuth tends to form unacceptably large crystallites upon solidifying from the melt. This project involved developing the exact metallurgical procedure (i.e., densifying finely crystalline Bi powder under the proper pressure and temperature) to synthesize this groundbreaking new filter. The neutron transmission of the Bi filter prototypes will be measured on the Disc-Chopper Spectrometer (DCS). The purity of the Bi materials will be monitored by neutron powder diffraction (NPD) and NVS.

University of Minnesota – Twin Cities

A Crossed-wire Molecular Electronic Test Structure

Curtis Mead

Molecular electronics is a field that may provide an alternative to conventional semiconductor devices and manufacturing, offering advantages such as cost savings through production by chemical synthesis, molecular uniformity with atomic precision, and device sizes not limited by lithographic processes. Essential to this field is the study of electrical properties of molecules. A system to conduct current-voltage measurements through gold-molecule-gold junctions has been constructed. The system consists of two 10um gold wires in a crossed-wire configuration, a magnet, a base to provide mechanical and electrical contacts, electronics for controlling the movement of the wires, and custom software to automate data acquisition. The crossed wire system achieves small-area molecular junctions by moving the molecule coated gold wires into electrical contact through the use of a precisely controlled deflection current in the wire that is orthogonal to the magnetic field.

Accurate Three Dimensional Graphs of Special Functions

Sheehan Olver

The Digital Library of Mathematical Functions (DLMF) is a project to update the ubiquitous, but aging, Handbook of Mathematical Functions (with Formulas, Graphs, and Mathematical Tables), which was originally published by NIST's predecessor the National Bureau of Standards in 1964. The DLMF will produce both a hardcover handbook, including mathematical advances made since the original handbook was released, as well as a web-based handbook to take advantage of modern computer technology. In addition to the material present in the hardcover handbook, the web-

based portion will contain math-aware searching, graphs in 2 and 3 dimensions, and other valuable resources.

One aspect of the DLMF is the creation of 3D visualizations of special functions. These visualizations are required to be accurate, in that they appear on screen exactly as they should and contain no false data points. They may also be clipped in cases where the function goes to infinity. All poles and other singularities must be plotted accurately. Finally, there is a limit on the number of sampled data points, as too many data points result in unnecessarily large files, and make manipulation extremely hard on slow machines.

In order to obtain smoothness with a small number of points, it is required to concentrate the grid in specific areas. In order to achieve this, we developed a system to concentrate a grid based on a given density function. By using second partial derivatives, we can construct a density function concentrated where the function is changing rapidly.

University of North Carolina – Charlotte

The World is Getting Smaller, Step by Step

Chad Bryant

As a result of advancing technologies and the decreasing size of devices there has become a high demand for micro- and nano-manufacturing. One avenue to reach this goal is through meso-scale machine technology. Meso, in a machining connotation is defined as the size scale between the micro and the standard scales. Instead of jumping directly from standard scales to micro- and nano-scales, this project takes the small step into meso-manufacturing. Eventually, in this incremental process, nano-manufacturing will be ascertained.

The Meso-Mill is an application of the meso-scale technology. The machine tool is designed to be a tabletop machine. The final design calls for five axes that will manufacture components of 50 mm^3 or smaller and reduce unnecessary repositioning of the part. For testing procedures, a three-axis prototype is explored. The prototype is controlled using PMAC, a motion control system. Calibrations were completed to determine the gain through the machine from input to output. The linear and angular error motions were measured to determine positioning errors of the part. The metrology set-ups to measure the error motions were designed and manufactured. These setups were unusual due to the unique configuration of the Meso-Mill's axes.

University of Notre Dame

Absorption Coefficient Measurements of Aerosol Particle Agglomerates
Steve Arico

Greenhouse effects associated with global climate change may be influenced strongly by the chemical and physical properties of particulate matter in the atmosphere. Currently, the largest uncertainty in environmental modeling is poor knowledge of the optical properties of atmospheric aerosols, such as atmospheric soot and cloud condensation nuclei. Although a variety of methods exist to measure atmospheric aerosol elemental carbon mass, those based on thermal-optical analysis (TOA) are the most widely used. TOA technology is deceptively simple, based on poorly understood, complex physical and chemical mechanisms. Current TOA methodology makes critical and untested assumptions about the thermal and optical behavior of particulate matter on a quartz fiber substrate, as well as the instrument-produced byproducts of pyrolysis.

To address these issues, it was necessary to create a thermally well-controlled environment in which to study particulate matter, and to devise a method of non-intrusive investigation. To this end, a laser-driver thermal reactor (heating at rates of up to 200 k/s), an acoustic levitator (removing the potentially spurious effects of heating a soot-bearing surface), and Stokes / Anti-Stokes Raman spectroscopy are being combined to determine the thermal-optical and chemical-kinetic properties of combustion-generated soot.

University of Puerto Rico

How Accurate are Calculations from Molecular Mechanics?
Claribel Acevedo

The field of computer simulation has enjoyed rapid advances in recent years. Computer simulations have a valuable role to play in providing exact results for chemical problems that would be intractable or even impossible via experimental methods. The rapid emergence of computational chemistry has impacted the work of all chemists and significantly increased efficiency in a number of fields.

To help this effort the NIST Computational Chemistry Group is developing databases and archives that are useful resources for scientists who want to compare their experimental data and theory in order to establish the accuracy and reliability of their experiments. This project is an extension of the Computational Chemistry Comparison and Benchmark Database, which is a website that allows users to compare gas-phase thermochemical properties from experiments and theory. This theory is mostly obtained from quantum chemical calculations. It includes enthalpies of formation,

entropies, geometries, vibrational frequencies and other data. The goal of the website is to answer the question "How accurate is that calculation?"

Since there are not that many ideal gasses out there, and there are many properties, such as viscosity, that quantum calculations cannot tackle, people use molecular mechanics to predict these properties .The molecular mechanical method uses balls and springs to treat atoms and bonds, respectively, in order to describe the bonds' ability to stretch, bend and twist. Molecular mechanics is much cheaper, so much larger molecules and intermolecular properties can be calculated, but since a lot of the physics has been left out, the accuracy question is even more relevant. As a result, we would like to include some molecular mechanics calculations in the CCCBDB, starting with the properties already present, such as geometries, using a variety of different ways of doing the calculations. In this project four force fields were compared: AMBER, OPLS, MM+, and BIO+. The goal of the project is to compare the accuracy and precision of these methods to experiments and to results from quantum calculations.

Ray Tracing of a Fourier Transform Spectrometer
Maria Casper

A Fourier transform spectrometer (FTS) measures the absorptions and emissions of any liquid, solid, or gas. ZEMAX is a lens design program that uses ray tracing to model refractive, reflective, and diffractive sequential and non-sequential optical systems. It is very time consuming and costly to run test after test of any matter through the FTS, thus the need for ZEMAX. The interferometer in the FTS was modeled part by part. First, the cats eye was modeled and then tested to see how sensitive tilting the angles of the primary and secondary mirrors and how changing the aperture size and the focus affected the system. The maximum tilt, aperture size, and focus were determined by analyzing the image and the wavefront map. Then, the interferometer without the beamsplitter was modeled to test the sensitivity of these types of changes. And finally, the interferometer with the beamsplitter was design, again to test its sensitivity.

NIST Work in Radiation Detection for Homeland Security Applications
Angel Fuentes-Figueroa

Since the attacks of September 11, 2001 the United States is trying to improve the security in every agency and public space. The battle against terrorism involves the development of new techniques that allow the early detection of possible threats. From all possible threats, the ones that include the use of radioactive materials or biological agents are of greatest concern. The development and use of detectors can lower and even eliminate the possible success of attacks. Standards are needed to ensure the acquisition and use of the right equipment for the intended purpose.

As part of a larger effort to improve scientific tools, such as radioactive detectors, experiments are being conducted at the National Institute of Standards and Technology (NIST) to investigate the functionality, detection limits and efficiency of a series of handheld detectors and portal monitors. Some examples of these detectors range from isotope identifiers, personal dosimeters, survey meters to portable portal and fixed portal monitors. Some of these radiation detectors are already being used at different sites by the United States Postal Service, Federal Express, United Parcel Service and Customs among other agencies. In an experiment that lasted three weeks, a portal detector was installed at the NIST C Gate in order to study the detector's behavior in a real time situation. Also as a major part of the research, handheld detectors responses were tested for ^{60}Co, ^{137}Cs and X-ray sources at different exposure rate values.

At ports and other facilities like airports and harbors where imported and exported products are carried in cargo containers, smuggling of radioactive materials is of great concern. With this in mind, at the NIST Cargo Container Facility we used a linear motion system to apply different speeds to sources like ^{133}Ba, ^{137}Cs, ^{152}Eu and ^{207}Bi with different activities and measure the detectors response as a function of the speed, γ-ray energy and activities level. All these experiments in conjunction with the development of new standards for homeland security applications will provide the U.S. government as well as the private sector with more efficient tools for evaluation and testing of radiation detectors used for detection of possible threats such as radiological dispersal devices (RDD) and nuclear materials.

Combinatorial Approach to Electrodepositing Copper-Cobalt Alloys

Emil Hernandez

Electrochemical methods are applied in research for different purposes. An example of this is the electro-deposition of alloys, of which mechanical and chemical properties vary from those of pure metals; hence they are of great utility. Our project goal was to develop a method that allows us to electrodeposit a wide range of alloy compositions on a single electrode by varying the potential distribution along the electrode. This is accomplished by varying the separation between the cathode and anode in the electrolyte. One should be able to predict the composition distribution with knowledge of the electrochemical kinetics of the individual electro-active components and the specific resistivity of the electrolyte. In order to do this, we used electro-analytical methods (e.g. cyclic voltammetry) to determine: 1) Diffusion coefficient (Do), 2) Exchange current Io and transfer coefficient a, and 3) Solution resistance. Once we established these mass transfer and kinetic parameters we calculated the composition distribution of a copper-cobalt alloy for a variety of cell geometries.

To determine the accuracy of our predictions, we electroplated copper-cobalt alloys from a sulphate-based electrolyte of known resistance under a predetermined potential distribution. This was realized in an electrochemical cell design in which the distance

between the electrodes (working and counter) increases, thus a potential gradient is created resulting in an alloy deposits of varied compositions. The deposits were then submitted to quantitative analysis by X-Ray Fluorescent measurements and Scanning Electron Microscopy.

Condition-based Monitoring of Equipment via Web-based Smart Sensor
Keriel Rodriguez

Smart Sensors and sensor networking are emerging technologies that will change the ways industry uses sensors. To help path the way, the smart sensor interface standard IEEE P1451 is established to provide a standardized method of accessing sensor data and Transducer Electronic Data Sheets (TEDS), a key component of the standard. The ability of accessing sensor data via the Internet allows remote monitoring equipment condition and industrial process anywhere in the world where an Internet hookup is readily available. This led to our idea of experimenting with an IEEE P1451.4-based accelerometer sensor and associated signal-processing unit and creating a custom web server that allow a client remotely access the sensor information. This project involved the understanding of the IEEE P1451.4 standard, smart sensor signal processing, software communication via dynamic link library (dll), the working of the Apache web server software, development of web server based on Apache, and the integration of sensor information to the web page.

University of Rochester

Protective Clothing Training Simulator
Long Nguyen

Knowledge of conditions that affect the thermal response of protective fabrics is crucial when considering actions that may place fire fighters in situations where their turnout gear fails to provide sufficient protection from fire exposures. A software package, the Protective Clothing Training Simulator, has been developed to bring this knowledge to the fire fighters and increase the level of awareness concerning conditions that may affect their garments and the protection offered. This package is a graphical tool featuring a simple interface that allows the user to set the degree of thermal insult, include the presence of trapped moisture and allow for the possibility of compression within a representative system of protective fabrics. The tool utilizes a simulation program with conditions collected from the user's input. Graphical feedback is presented to the user in the form of an animated graph. Through the graph, the user will be able to see, as time progresses, the inner and outer surface temperatures of a turnout garment, the skin surface temperature and predictions for the onset of first and second-degree burns. The results illustrated by the graphical tool, complemented by a

structured training plan, will provide a better understanding of how turnout garments respond to fire exposures.

University of Texas – Austin

Development and Construction of a Thermally-Driven Outdoor Sealant Testing Device

Joseph Fradella, III

An outdoor-exposed, thermally-driven device was constructed to measure the stress and strain response of sealant samples. This device involves a rigid frame of wood and steel connected to a pair of PVC pipes that drive the motion of the sealant samples. Such a configuration is designed to simulate the thermally-induced fatigue cycles of sealant in a commercially-constructed building.

Load cells measure the amount of stress on each sample, while Linear Variable Differential Transformers (LVDT) gauge the strain on the samples. This data is processed through a data acquisition system and is recorded to allow for analysis of sealant stress-strain response to changes in temperature.

In order to determine the length of pipe needed to produce the desired sealant strain, the coefficient of thermal expansion for PVC was calculated and verified against an accepted range of values. The frame is constructed such that the only source of motion is the PVC pipe. The device was filled with a water-ethylene-glycol mixture and tested over the expected outdoor thermal range using a rigid steel sealant sample in order to determine the compliance of the entire system. This data, along with the placement of turnbuckles along the sample shafts, allows for accurate measurement of sealant strain.

The stress-strain data collected from this device over the next several years is part of a larger effort in service life prediction of building materials.

University of Washington

Effects of Transverse Coupling on the Fragmentation of a Bose-Einstein Condensate in a Double-well Potential

Heidi Perry

The Bose-Einstein condensate (BEC) is a new form of matter, first created in 1995. It is a quantum mechanical system large enough to be seen with the naked eye and is of great interest to both theoretical and experimental physicists because it allows for the exploration of quantum mechanical properties on a mesoscopic scale. The possibility that a dilute gas of atoms could all enter the same wave function was predicted by Albert Einstein and Satyendra Nath Bose in 1924, but the difficulty in obtaining a

temperature low enough for atoms to undergo this phase transition delayed the experimental realization of this phenomenon. I will present the results of a theoretical study of the Bose-Einstein condensate in a double-well potential coupled to a two-dimensional harmonic oscillator in the transverse plane. The BEC in a one-dimensional double-well is a well studied system. In the limit of a low barrier between the wells, the system is in a coherent state where particles are free to tunnel between the wells; as the barrier is raised, tunneling is quenched and the system fragments into two distinct condensates. We are interested in the effects of the coupling of the double-well to the transverse degrees of freedom on the energy level spectrum and the transition from a coherent to a fragmented regime.

Ursinus College

Design and Synthesis of a DNA-binding Protein Module
Salita Kaistha

Proteins that bind specific DNA sequences can yield valuable information on the structural basis of their binding, in addition to serving as tools for DNA analysis and as modules for nanoconstruction. The transcription factor Max (PDB ID: 1AN2) was selected as a test system for specific modification and synthesis. The protein architecture was modified by truncation to its 51 N-terminal amino acids (which include the DNA-binding domain) with 4 other specific replacements. The modified gene was synthesized de novo by PCR methods, cloned into E. coli, and expressed. Ongoing work hopes to show that the purified protein will dimerize and bind the target duplex DNA sequence. This would confirm the efficacy of the design and synthesis methods, and would suggest the possibility of making proteins with tailored capacities for molecular assembly.

Vanderbilt University

Electroplating Fabrication Approach to Nanometer-Scaled Fluidic Restrictions
Melanie Bernard

Nanometer-scaled restrictions are among the latest devices being researched for their capability to detect small particles, especially DNA. Silver was electroplated onto the surface of pores that were micromachined in silicon substrates to reduce their size to nanometer dimensions. Plated samples were evaluated by optical and electron microscopy to determine the effect of different plating methods. It has been proposed that pores spanning a few nanometers can be used as structures through which to thread individual polynucleotide molecules by applying a potential across the pore. As the molecule passes through the hole, fluctuations in the current might detail each base and thus be used to rapidly sequence small quantities of DNA. To explore this approach, solution phase conductivity tests were performed.

A photolithographic and wet etch fabrication procedure was used to form micrometer-scaled holes in silicon wafers. Silver ions in the plating solution were electrochemically reduced to form crystal clusters around the opening. Different plating parameters were tested including length of time and amount of potential applied. The optimal plating method was determined to be a continuously applied potential between –50 mV and -125 mV (vs. Ag reference electrode). The magnitude of the applied potential could vary within this range and still produce pores of similar size and quality. It was determined that the quality of plating and pore dimension varied widely among similar-sized samples even though experimental conditions were identical. Pores with desirable characteristics could be produced, but further development is required to improve the yield. Following fabrication, ionic conductivity across the silver-plated structures was used to detect the presence of restrictions too small to be observed with optical microscopy. Ionic conductivity data also indicated the presence of obstructions, such as gas bubbles, inside the apertures. Pores of various sizes underwent testing to determine a relationship between pore area and ionic conduction. The data suggest a need to revise the experimental procedure before ionic conductivity can be used to quantify the open areas of the pores.

Spatially Controlled Biomolecular Deposition in Microfluidic Systems

Hilary Samples

The miniaturization of chemical analysis and detection systems continues to be at the forefront of scientific and technological research with the hope of developing effective 'Lab-on-a-chip' technologies. Such systems can be realized using microfluidic methods to create microchannel devices and micropatterned arrays in which numerous biochemical reactions and processes can occur. These devices contain surface characteristics that allow for the specific immobilization of such biomolecules as DNA, proteins, antibodies, and enzymes, all of which hold great promise for future applications. This presentation will demonstrate the procedures of microfluidic device fabrication, chemical deposition and micropatterning. Together, these techniques constitute the abilities to manipulate the functional surfaces of polymers and to selectively control the adsorption of molecules within such devices. In this research,

microchannels are coated with protein, patterned with UV laser ablation, subjected to specific biomolecular deposition, and in effect, designed to selectively bind materials of interest in a controlled, spatial pattern in microfluidic devices.

Adaptive Control for the Enhanced Machine Controller
Matthew White

Today's manufacturers demand high-precision, high-versatility CNC controllers to drive the machine tools that make parts for the automotive, aerospace, and many other industries. Because commercially available closed-architecture controllers are expensive and cannot be easily maintained or upgraded, many smaller machine shops employ free, open-architecture controllers such as NIST's Enhanced Machine Controller (EMC). As part of an ongoing effort to further develop the capabilities of the EMC, experiments were conducted to investigate the possibility of adding adaptive control features. Using Hall effect sensors to measure the current and power being supplied to the drive motor, it is possible for the controller to determine the load on the spindle at any point during a machining process. The load on the spindle can tell us many useful things about the machining process, such as when the tool bit wears down or breaks, when the tool is entering or exiting the work piece, or when the tool encounters a hard spot in the material. Using this load information, the controller can automatically adjust the feed rates and spindle speeds, enabling manufacturers to achieve maximum productivity while still ensuring safety and quality.

Western New England College

Optical Tweezers for Nanomanufacturing
Craig Beal

Functional MEMS devices have been produced using the standard layering processes of IC fabrication, however success has been limited at the nanoscale, indicating that the realization of nanotechnology calls for more than further minaturization of current technology and techniques. We propose to manufacture each component separately, cause them to lift off their substrate, and assemble them in a new location. Such a method would allow for non-planar realative component orientations that should provide added functionality and in many cases a simplifed design.

However, the nature of the nanoscale environment limits our ability to mechanically manipulate matter and forces us to explore new avenues. The development of an instrument, called optical tweezers, uses photon momentum to induce comparatively large forces on small particles that may be suspended in a solution or electrostatic field. In this presentation, the audience will gain an understanding of the proposed nanomanufacturing process and the basic physics of optical trapping. The design of an

optical tweezers based on a Linnik interferometer will be covered in detail and the discussion will conclude by touching upon how the information gained from this instrument will be applied to the development of a much more advanced instrument with an intuitive interface.

Extensible Markup Language for Data Storage and Retrieval
Alan King

Sensors that provide pertinent data about object or spatial conditions often have different forms of storing that data. This lack of structure makes data retrieval difficult for single or multiple applications that may need to access the data from different sensors to perform a function.

The Construction Metrology and Automation Group is using a position sensor to locate construction components, specifically steel beams and beam holders, within a construction site. The software that stores the data, however, does not provide descriptive information about that data, which may be useful to applications that may need to use the information for functions such as crane operation or real time modeling. In order to provide a better description of and information on how to read the data, the data file is reformatted using extensible markup language (XML). An application can access the new XML document, determine how the file is to be read and retrieve the necessary data to perform a function. Using XML not only allows multiple applications to access and retrieve data specific to the application, but by specifying how to read the file, allows a single application to access data files with different formats.

Western Washington University

A Self Balancing Power Calibration System
Casey Hardy

The electric power industry generates revenues of more than $240 billion annually. It requires the accurate measurement and monitoring of electric power to ensure the equitable sale of electric energy to U.S. consumers. NIST supports the industry by offering high precision calibrations in the areas of power and energy measurement.

The research conducted dealt with the verification of a self-balancing power calibration system. This system was purchased commercially and is intended to replace an older calibration system currently being used at NIST. Unlike the older system, the new one utilizes a self-balancing power bridge and therefore eliminates the time consuming process of manually balancing the bridge when performing meter calibrations. The testing of the new system involved extensive data acquisition with numerous wattmeters/watt converters. Error and uncertainty analysis of the acquired data were then performed along with the comparison of other systems within NIST.

Not only would the implementation of this new power calibration system be cost-effective, but it would also significantly decrease the amount of time needed for meter calibrations and in turn greatly reduce the turn around time of the customer's product.

Williams College

Two-beam Diffraction Patterns in a Nonlinear Medium

Aubryn Murray

When two laser beams are overlapped in a nonlinear medium, a pattern is observed that is distinctly different from the individual diffraction pattern of either beam. The circular rings of the single beam pattern are replaced by "D"-shaped rings. This effect is produced by cross-phase modulation. It was observed in liquid crystals and in Rb vapor near resonance. Variation of the effect with beam curvature and overlap were investigated and reproduced in computer-generated models.

Worcester Polytechnic Institute

Crack Growth Studies in Indium Phosphide

Brian Cordes

The research done this summer is directed towards lifetime predictions in semiconductors, specifically Indium Phosphide (InP). Lifetime prediction is defined as the probability that a specimen or component will retain structural integrity under an applied stress for a specified time. For accurate lifetime predictions, it is necessary to know both the initial strength and the strength degradation rate of the material. This summer we are focusing on the strength degradation aspect of the lifetime prediction. Strength degradation, i.e., slow crack growth, has been extensively studied in oxide materials, resulting in a model that explains bond rupture (crack growth) as a function of stress. However, previous work on Si, GaAs, and InP suggests that this model is not applicable to semiconductors. In particular, no functional relationship between load and crack velocity has yet been found for InP.

In this work, rectangular specimens were cleaved from InP wafers. Cracks were initiated in each specimen using a diamond indenter in a mechanical test machine; the stiffness of the machine allowed stable crack initiation, i.e., crack formation without specimen failure. Specimens were tested under two different loading configurations; the first applying primarily tensile stresses and the second applying primarily shear stresses to the specimen. Crack extension was observed on specimens under both loading configurations. Qualitative crack velocity measurements have been made as a function of time for various applied loads. Optical microscopy was used *in situ* to

monitor crack growth in real time as well as post-test to observe features along crack walls. The cracks were observed to stop running in both configurations while still under load. Locations at which crack growth stopped were marked on the specimen for *post-mortem* examination. To interpret our results, we intend to use the orientation imaging capability on an available SEM to investigate whether dislocations play a part in the observed crack arrest. We also intend to apply fractography techniques and atomic force microscopy to investigate the fracture surfaces. Our goal is to determine the mechanisms that cause crack growth and crack arrest in these materials.

APPENDIX A. A QUICK CROSS-REFERENCE – SURF 2003

SCHOOL	STUDENT (last/first name)	PROJECT TITLE	NIST LAB	PAGE
American University	Casey, John Patrick	Automation of Ionizing Radiation Measurements	PL	19
Appalachian State University	Cass, Matthew	An Investigation Into Current Residential Fire Codes in Regards to Safety	BFRL	19
Appalachian State University	Naff, Jessica	Defining the Relationship Between Surface Composition and Protein Adsorption	CSTL	20
Appalachian State University	Robertson, Erin	Surface Properties of Imidazoline Surfactants	MSEL	20
Appalachian State University	Stamilio, Rebecca	Determining Minority Carrier Diffusion Length of GaN Using Surface Photovoltage Spectroscopy	EEEL	21
Brown University	Chun, Melissa	Analysis of Ozone-enhanced Oxidation for Device Passivation Layers	EEEL	21
Brown University	Riechl, Patrick	EMC Threading	MEL	22
Bryn Mawr College	Philip, Mary	Evaluation of a Novel Moisture Transport Model for Epoxies and Sealant Materials	BFRL	22
Bucknell University	Paoletti, Matthew	Characterization of Bioencapsulated Proteins	MSEL	23
California Polytechnic State University – San Luis Obispo	Chau, Kour Thay	Evaluation of (VUV-SE) Ellipsometer and Optical Properties of High-k Hafnium Aluminate Oxides	EEEL	23
California State University – Sacramento	Morris, Eliza	Locking to Absorption Lines for Laser Spectroscopy	PL	24
Carnegie Mellon University	Kim, Daniel	Creating a Web-based Aid to Monitor NIST and Customer Standards	EEEL	25
Carnegie Mellon University	Velazquez, Amanda	Polymorphic Phase Transitions in the SrO-Li_20-Nb_2O_5 System	MSEL	25
Case Western Reserve University	Langhorst, Ben	Optical Study of Shear-Induced Structure of Polymer-Dispersed Carbon Nanotubes	MSEL	26
City College of New York – Hunter College	Jackson, Randy	The Study of Nanofabricated Surfaces for Protein Immobilization	CSTL	26
Clemson University	Ferguson, Erin	Studying Particle Release Induced by Air Jets: A Critical First Step in Explosive Particle Detection for Airport Security	CSTL	27
Clemson University	Luedeke, Katelyn	Lightweight MgLi Alloys: The Future of Automotive Research	MSEL	27
College of William and Mary	Small, Samuel	A Starvation-Free Preference-Based Job Scheduler for the ScreenSaver Science Project	ITL	28
Cornell University	Robinson, Jennifer	Preparation and Characterization of Nanostructured Surfaces for Surface Enhanced Raman Spectroscopy (SERS)	PL	29
Davidson College	Scott, Gregory	Comparison of Computational Methods for Electron-Impact Ionization Cross Sections	CSTL	29
Drexel University	Bespalov, Dmitriy	Automated Software Integration	MEL	30
Drexel University	Kopena, Joe	Semantic Integration Through Invariants	MEL	30
Duke University	Chang, Daphne	Measuring the Neutron Lifetime Using Magnetically Trapped Ultracold Neutrons	PL	31
Fordham University	Halt, Olivia	Absolute Radiometry with Correlated Photons	PL	32
Gettysburg College	Anderson, William	Fast Neutron Spectroscopy	PL	33
Hamilton College	Auerbach, Ben	Transmittance of Fused Silica (SiO_0) Windows	PL	33
Harvard University	Maliaris, Constantin (Ted)	Temperature Gradient Focusing for the Separation of Proteins	CSTL	34
Iowa State University	Holzmueller, Jason	Chemical Modification of TiO_2 Nanoparticles for the Improvement of Dispersion in Acrylic Urethane Polymer Matrices	BFRL	34

SCHOOL	STUDENT (last/first name)	PROJECT TITLE	NIST LAB	PAGE
James Madison University	Muth, Jennifer	Synthesis of X-Ray Photoelectron Spectroscopy Lineshapes Using MATLAB	CSTL	35
James Madison University	Schwartz, Evan	Augmentation of Biopolymers for Tissue Engineering	MSEL	36
Johns Hopkins University	Lee, Joe	An Investigation into the Corrosion Resistance of High Nitrogen Stainless Steel	MSEL	36
Johns Hopkins University	Rockwell, Andrew	Analysis of Cell Membrane Peptides Via Small Angle Neutron Scattering	MSEL	37
Kent State University	Stemen, Kyle	Computational Material Science Software Development	MSEL	37
Lehigh University	Chumakov, Marina	Strength of Silicon in the Region of Small-Scale Flaws	MSEL	38
Loyola College	Watts, Stacey	The Creation of a Successful Imaging System: A Step in Improving the Way We Study Plasma Arc Tubes	PL	39
Marietta College	Avery, Seth	Corrosion as a Mechanism of Crack Tip Blunting in Glass	MSEL	39
Massachusetts Institute of Technology	Handler, Matthew	Flow Simulation for the Development of Microfluidic Devices	MSEL	40
Massachusetts Institute of Technology	Tang, Iris	A Study of the Bystander Role in HRI	ITL	40
Miami (Ohio) University	O'Connor, Kathryn	Development of a Second Generation Domen-type Water Calorimeter as a Primary Standard for Absorbed Dose in a ^{60}Co Beam	PL	41
Miami (Ohio) University	Seymour, Bobby	Atomic Resolution Electromechanical Null Detection	MEL	41
Michigan Technological University	Gillespie, Justin	Ensuring the Consistency of World Model Knowledge in Autonomous Navigation	MEL	42
Montgomery College	Dafla, Hiruy T.	Determination of the PSD of Gypsum in Cement	BFRL	42
Mount Saint Mary's College	Daschbach, Megan	The Ultraviolet Absorption Cross Sections of 1,5-Hexadiyne: Temperature Dependent Gas Phase Measurements	CSTL	43
Mount Saint Mary's College	Kalema, Anna	Degradation of PCBs in Marine Sediment by Electron-Beam Technology	CSTL	44
North Carolina State University	Hill, Ryan	Improving the Performance of Point-of-Care and Bio-Warfare Detection Methods that Use Portable Fluorescence Spectrometers	CSTL	44
Oregon State University	Maunder, Cary	Development of Simulation of Job Shop Processes	MEL	45
Pomona College	Ban, Han Yong	Spectroscopy of Er for Cooling and Trapping Purposes	PL	45
Princeton University	Molino, Van John	A Differential Equation Approach to the Determination of the DMA Transfer Function	ITL	46
Reed College	Hopkins, Elizabeth	Structure, Chemistry, and Dielectric Properties of $Ba_3MgSb_xNb_{2-x}O_9$ and $Ba_3NiSb_xNb_{2-x}O_9$ Ceramics	MSEL	47
Rensselaer Polytechnic Institute	Lippiatt, John	Optical Tweezers Tip-Tilt Mirror Analysis	MEL	47
Rensselaer Polytechnic Institute	Lippiatt, Sherry	The Use of Real-Time Polymerase Chain Reaction in Quantifying Inflammatory Responses to Biomaterials	MSEL	48
Rensselaer Polytechnic Institute	Matarazzo, Mark	Towards Attofarad (10^{-18}F) Capacitance Measurements: A Comparison of Capacitance Sensor Designs	EEEL	48
Rhodes College	Diez, Dustin	Selective Electro-deposition of Actinides	PL	49
Rochester Institute of Technology	Crigger, Lara	Properties of Polymersomes: A Practical Use of the Optical Tweezers and Scalpel	PL	50
Saint Joseph's University	Scheuermann, Joshua	Prostate Cancer Seed Calibration and Characterization	PL	50
Saint Mary's College of Maryland	Rafferty, Ian	Flame Size vs. Heat Release Rates	BFRL	51
Santa Monica College	Kangavari, Peyman	CMOS MEMS Test Structures for the Measurement of Young's Modulus	EEEL	51
Santa Monica College	Kim, Therasa	Methodologies for Measurement of TiO_2 Photoreactivity	BFRL	52
Santa Monica College	Shin, Ji-Young	Concrete Microstructure and Aggregate Shape on the Millimeter Scale	BFRL	52

SCHOOL	STUDENT (last/first name)	PROJECT TITLE	NIST LAB	PAGE
Southern Methodist University	Britton, Mackenzie	Autonomic Service Registration for the Service Location Protocol	ITL	53
Southern Methodist University	Skaggs, Alan	Ferromagnetic Resonance in Thin Magnetic Films	MSEL	54
State University of New York – Binghamton	Chen, Shi Zhi	Mapping eBusiness Specifications	EEEL	54
Tougaloo College	Rainey, Jr., Julius	Advancement in Construction Site Technologies	BFRL	55
Tulane University	Broussard, Leah	Systematic Studies in the emiT Time Reversal Violation Experiment	PL	56
Tulane University	Wiener, Alexander	Radiative Decay of the Neutron	PL	56
University of California – Berkeley	Krivulina, Liliya	Planning on Traffic Growth in Optical Access Networks	ITL	56
University of California – Berkeley	Lee, Jonathan	Interferometry: PSI and VSI Discrepancies	MEL	57
University of California – Berkeley	Wong, Iris	Integration of Microcontroller for Embedded Gas Sensor System-on-a-Chip	EEEL	57
University of California – Irvine	Duong, Tam Hoang	A New IMPACT in Silicon Carbide Power MOSFETs	EEEL	59
University of California – Irvine	Esiobu, Adaeze	Binary Analysis of High Volume Data Sets	ITL	59
University of California – Irvine	Garg, Akash	Verifying and Standardizing Functionality of Forensic Hardware Devices	ITL	60
University of California – Irvine	Liang, May	"In Search of a Hot Pig" – Thermal Detection of Radioactive Materials	PL	61
University of California – Irvine	Nguyen, Alice	Temperature Control in the Molecular Measuring Machine	MEL	62
University of California – Irvine	Patel, Ravi	A Method to achieve CD Reference Materials with 100 nm Linewidths	EEEL	62
University of California – Irvine	Sanders, Jamaal	The Kinetics of Cluster Formation of Polyethylene Oxide in Water	MSEL	63
University of California – Irvine	Varghese, Shalini	Depth Profiling of Polymeric Samples Using SF_5^+ Primary Ion Bombardment	CSTL	63
University of California – Irvine	Zhang, Eric	Visualization and Segmentation of Objects Based on Riegl Data	MEL	64
University of Colorado – Boulder	Scheib, Jennifer	Characterization of LED Power Distributions	PL	65
University of Kentucky	Lane, Andrew	Stimulating Quantum Circuits at the Gate-Level: QCSim	ITL	65
University of Maryland – Baltimore County	Adedeji, Aolat	Digital Rights Management	ITL	66
University of Maryland – Baltimore County	Powers, Michael	Modeling Near-Interfacial Defects in High-k Dielectrics	EEEL	66
University of Maryland – Baltimore County	Vicente, Marcos	Plasma Diagnostics for a Dual Frequency Plasma Source	PL	67
University of Maryland – Baltimore County	Walsh, Thomas	VOIP Security	ITL	67
University of Maryland – College Park	Anderson, Kelly	Organic Monolayers on Silicon(111)	CSTL	68
University of Maryland – College Park	Downs, Anthony	Air-Ground Sensor Registration	MEL	69
University of Maryland – College Park	Feldman, Kiri	X-Ray Absorption Measurements of Water Loss in Curing Mortar Samples	BFRL	69
University of Maryland – College Park	Kratchman, Jessica	Modeling Smoke Detectors	BFRL	70

SCHOOL	STUDENT (last/first name)	PROJECT TITLE	NIST LAB	PAGE
University of Maryland – College Park	Mehraban, Shirin	Studying Protein Sequences Using Bioinformatics	ITL	70
University of Maryland – College Park	Quarrick, Timothy	Sheet Metal Studies on Fe-base Alloys	MSEL	71
University of Maryland – College Park	Su, Richard	Performance and Cost Tradeoffs for Use of Omni-directional vs. Unidirectional Regenerators in Optical Networks	ITL	71
University of Maryland – College Park	Yeung, Chiu	Testing for the Common Intersection Point of Lines	ITL	72
University of Maryland – College Park	Zeitoun, Ramsey	Development of a Bismuth Filter for Neutron Vibration Spectroscopy	MSEL	72
University of Minnesota – Twin Cities	Mead, Curtis	A Crossed-wire Molecular Electronic Test Structure	EEEL	73
University of Minnesota – Twin Cities	Olver, Sheehan	Accurate Three Dimensional Graphs of Special Functions	ITL	73
University of North Carolina–Charlotte	Bryant, Chad	The World is Getting Smaller, Step by Step	MEL	74
University of Notre Dame	Arico, Steve	Absorption Coefficient Measurements of Aerosol Particle Agglomerates	CSTL	75
University of Puerto Rico	Acevedo, Claribel	How Accurate are Calculations from Molecular Mechanics?	CSTL	75
University of Puerto Rico	Casper, Maria	Ray Tracing of a Fourier Transform Spectrometer	PL	76
University of Puerto Rico	Fuentes-Figueroa, Angel	NIST Work in Radiation Detection for Homeland Security Applications	PL	76
University of Puerto Rico	Hernandez-Pagan, Emil	Combinatorial Approach to Electrodepositing Copper-Cobalt Alloys	MSEL	77
University of Puerto Rico	Rodriguez, Keriel	Condition-based Monitoring of Equipment via Web-based Smart Sensor	MEL	78
University of Rochester	Nguyen, Long	Protective Clothing Training Simulator	BFRL	78
University of Texas – Austin	Fradella, III, Joseph	Development and Construction of a Thermally-Driven Outdoor Sealant Testing Device	BFRL	79
University of Washington	Perry, Heidi	Effects of Transverse Coupling on the Fragmentation of a Bose-Einstein Condensate in a Double-well Potential	PL	79
Ursinus College	Kaistha, Salita	Design and Synthesis of a DNA-binding Protein Module	CSTL	80
Vanderbilt University	Bernard, Melanie	Electroplating Fabrication Approach to Nanometer-Scaled Fluidic Restrictions	EEEL	80
Vanderbilt University	Samples, Hilary	Spatially Controlled Biomolecular Deposition in Microfluidic Systems	CSTL	81
Vanderbilt University	White, Matthew	Adaptive Control for the Enhanced Machine Controller	MEL	81
Western New England College	Beal, A. Craig	Optical Tweezers for Nanomanufacturing	MEL	82
Western New England College	King, Alan	Extensible Markup Language for Data Storage and Retrieval	BFRL	82
Western Washington University	Hardy, Casey	A Self Balancing Power Calibration System	EEEL	83
Williams College	Murray, Aubryn	Two-beam Diffraction Patterns in a Nonlinear Medium	PL	84
Worcester Polytechnic Institute	Cordes, Brian	Crack Growth Studies in Indium Phosphide	MSEL	84

BFRL – Building and Fire Research Laboratory, CSTL – Chemical Science and Technology Laboratory, EEEL – Electronics and Electrical Engineering Laboratory, ITL – Information Technology Laboratory, MEL – Manufacturing Engineering Laboratory, MSEL – Materials Science and Engineering Laboratory, PL – Physics Laboratory.

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